

Article

Péclet-Number-Controlled Solute Transport Regimes in Idealized Rough Rock Fractures: Implications for Groundwater Contamination

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Abstract

Solute transport in rock fractures is strongly influenced by hydrodynamic conditions, and clarifying the Péclet-number-controlled transition of transport regimes is important for understanding contaminant migration in fractured aquifers. Based on three-dimensional numerical simulations, this study investigates conservative solute transport in idealized rough fractures with perfectly mated walls and uniform aperture under a wide range of Péclet numbers (Pe). The evolution of concentration fields, breakthrough curves (BTCs), and diffusive and advective fluxes was analyzed to identify the dominant transport regimes. The results show that, as Pe increases, solute transport changes from a diffusion-dominated regime ($Pe < 0.1$), to a mixed macro-dispersion-dominated regime ($0.1 < Pe < 1000$), and finally to a high- Pe advection-controlled regime with Taylor-dispersion-like characteristics ($Pe > 1000$). Correspondingly, the concentration field evolves from rapid diffusion-driven spreading to a sharper advective front, while the BTCs change from early diffusion-breakthrough curves to step-like breakthrough behavior. Fracture aperture promotes solute spreading and broadens the mixing zone, especially under low-to-intermediate Pe conditions. In contrast, under the perfectly mated and uniform-aperture fracture conditions considered here, increasing roughness mainly induces local tortuosity of the concentration front and has limited influence on the overall BTCs. Flux decomposition further confirms that diffusive flux dominates at low Pe , whereas advective flux becomes increasingly dominant as Pe increases. These findings provide a mechanistic basis for interpreting Pe -controlled solute transport in idealized fracture channels and offer fracture-scale insights for classified groundwater contamination risk assessment. The implications should be interpreted within the assumptions of conservative transport without matrix diffusion, adsorption, or reactive processes.



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1. Introduction

Rock fractures are widely recognized as preferential pathways for subsurface fluid migration and solute transport. They commonly occur in various geological and engineering settings, including mining operations [1–4], geological disposal of nuclear waste [5,6],

and groundwater contamination scenarios [7–9]. Compared with intact rock matrices, fractured media generally exhibit much higher permeability and stronger transport heterogeneity [10]. Once contaminants enter fracture-controlled flow systems, they may migrate rapidly through connected fracture pathways, thereby affecting contaminant plume spreading, remediation efficiency, and pollutant leakage risk assessment [11,12]. Therefore, accurately understanding solute transport mechanisms in rock fractures is of great importance for predicting contaminant migration and developing effective groundwater protection and remediation strategies.

Solute transport in fractures is governed by the coupled effects of advection, molecular diffusion, and hydrodynamic dispersion [13]. Molecular diffusion is driven by concentration gradients, whereas mechanical dispersion arises from velocity variations and advective mixing during fluid flow. These processes jointly determine the spatial distribution of solute concentration, the morphology of transport fronts, the shape of breakthrough curves, and the temporal evolution of solute flux. Mechanical dispersion can be further classified into macro-dispersion and Taylor dispersion, depending on the dominant flow and mixing conditions [14]. The relative importance of advection and diffusion is commonly characterized by the dimensionless Péclet number (Pe), which represents the ratio of advective transport to molecular diffusion. As Pe varies, the balance between diffusion and advection changes, leading to different transport regimes and breakthrough behaviors.

The principal methods employed to investigate solute transport behavior in rock fractures include experimental studies [14–17], analytical approaches [18–20], numerical simulations [21–23], and, with advances in computational capabilities, machine learning techniques [24]. Recent coupled numerical studies have further emphasized the importance of resolving rough-fracture geometry and multi-factor hydraulic–mechanical effects when simulating subsurface flow and water-related hazards in mining environments. These studies indicate that fracture geometry, hydraulic conditions, and coupled physical processes may jointly influence fluid migration and transport behavior. Therefore, numerical simulation remains an effective approach for isolating key controlling factors and identifying dominant transport mechanisms in fractured media. Early investigations were predominantly based on parallel-plate models, using analytical methods or simplified numerical simulations to examine solute transport under idealized geometric and hydraulic conditions [25]. Detwiler et al. elucidated the relative importance of Taylor dispersion and macro-dispersion in fractures, demonstrating that their contributions to solute breakthrough behavior vary with the Péclet number [14]. Solute transport through fractures generally exhibits non-Fickian characteristics, such as early arrival and long tailing [26], and such non-Fickian behavior becomes increasingly pronounced with increasing Pe and Reynolds numbers [27]. With increasing Reynolds number, recirculation zones generated within the flow field may evolve from a rapid growth stage, through a slow growth stage, to a fully developed stage [28]. These enlarged recirculation zones can trap solutes and subsequently release them back into the main flow channel, resulting in non-Fickian transport characterized by bimodal or even multimodal breakthrough curves (BTCs) [29,30].

Fracture geometry is another key factor controlling solute transport behavior. Studies focusing on solute transport in rough fractures have shown that fracture wall roughness can alter velocity distributions and solute migration pathways [31,32]. Under Darcian flow conditions, roughness-induced boundary effects may modify the velocity distribution within the fracture, thereby affecting solute transport behavior. Under non-Darcian flow regimes, in addition to the altered velocity distribution, the increased volume of recirculation zones and the enhanced mass transfer rate induced by boundary effects may further influence solute transport [33]. The pronounced tailing phenomenon observed during solute transport in fractures can be attributed to complex internal heterogeneities [34].

Shear displacement-induced changes in fracture geometry may lead to aperture heterogeneity and preferential flow paths [35], thereby significantly altering the fluid vorticity field, solute-front morphology, and breakthrough time [36,37]. The mixing and partitioning patterns of solutes at fracture intersections during shear are controlled by shear-induced dilation [38], and increasing the contact ratio of intersecting fractures can intensify the tailing phenomenon of non-Fickian solute transport. Furthermore, intersection anisotropy and void-structure variations influence the redistribution and mixing of fluids and solutes [39]. It should be noted that the influence of roughness on solute transport is often coupled with aperture heterogeneity, shear displacement, contact-zone development, and preferential flow paths in natural fractures. Therefore, distinguishing the effect of wall roughness itself from the effect of aperture heterogeneity remains an important issue in numerical studies of fracture-controlled transport.

Although previous studies have greatly improved the understanding of solute transport in fractured media, several limitations remain. The role of Pe in solute transport has been widely recognized, but the integrated evolution of concentration-field morphology, breakthrough-curve behavior, and diffusive/advective flux contributions over a broad Pe range remains insufficiently clarified within a single rough-fracture framework. In addition, the conditional roles of fracture aperture and wall roughness under idealized geometric assumptions require further examination, especially when roughness is isolated from shear-induced aperture heterogeneity and contact-zone effects. For groundwater contamination assessment, such an integrated framework is useful because different hydrodynamic regimes may correspond to different contaminant spreading patterns, monitoring requirements, and remediation strategies.

To address these issues, this study employs three-dimensional numerical simulations to investigate conservative solute transport in idealized rough fractures under varying hydrodynamic conditions across a wide range of Pe values. The fracture models considered here have perfectly mated upper and lower walls and spatially uniform apertures, which allows the effects of Pe , aperture, and wall roughness to be examined under controlled geometric conditions. The specific objectives of this study are as follows: (1) to reveal the staged characteristics of the continuous evolution of solute transport mechanisms as Pe increases and to identify the Pe intervals associated with diffusion-dominated, macro-dispersion-dominated, and high- Pe advection-controlled transport with Taylor-dispersion-like characteristics; (2) to establish the relationships among concentration-field evolution, breakthrough-curve morphology, and diffusive/advective flux behavior; (3) to examine the conditional effects of fracture aperture and wall roughness on solute transport under different Pe conditions; and (4) to discuss fracture-scale implications for classified groundwater contamination prevention and control under conservative transport assumptions. This study provides a mechanistic basis for interpreting Pe -controlled solute transport in idealized rough fractures and supports the development of zonal groundwater contamination risk assessment strategies.

2. Method

2.1. Development of Fracture Model

Fracture surfaces in nature typically exhibit characteristic roughness and self-affine properties, which have been demonstrated to be reproducible through fractional Brownian motion [40]. Commonly employed methods for generating rough fracture surfaces include the Weierstrass–Mandelbrot (W–M) function method [41], the Successive Random Addition (SRA) method [4,42], and the spectral method [43]. Among these, the SRA method has been widely adopted owing to its high computational efficiency. In two-dimensional SRA, a single-valued continuous function $[a(x + \Delta x, y + \Delta y) - a(x, y)]$ is used

to describe the height distribution of the rough surface, which is defined as obeying a Gaussian normal distribution with a mean of zero and a variance of σ^2 over a distance of $l = \sqrt{(\Delta x)^2 + (\Delta y)^2}$. The height distribution of a self-affine fracture surface is defined by the following function [44,45]:

$$\langle a(x + \gamma\Delta x, y + \gamma\Delta y) - a(x, y) \rangle = 0 \quad (1)$$

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

where $\langle \cdot \rangle$ denotes the mathematical expectation, γ is a constant, H is the Hurst exponent ranging from 0 to 1, and σ^2 is the variance.

By setting different Hurst exponents (0.35, 0.4, and 0.45), three rough fracture surfaces were generated, as shown in Figure 1a,c,e. Figure 1b,d,f present the corresponding height distribution histograms of the fracture surfaces, from which it can be observed that the fracture surface height distributions conform to typical Gaussian distribution characteristics ($R^2 = 0.99$). To quantify the roughness characteristics of the fracture surfaces, the joint roughness coefficient (JRC) was calculated based on the root mean square of the first derivative of the fracture profile (Z_2) [46]:

$$Z_2 = \sqrt{\frac{1}{n-1} \sum_{i=1}^{n-1} \frac{(z_{i+1} - z_i)^2}{x_{i+1} - x_i}} \quad (3)$$

$$JRC = 32.2 + 32.47 \log Z_2 \quad (4)$$

where x denotes the coordinate of the fracture profile along the longitudinal direction, z denotes the coordinate along the height direction, n is the total number of data points, and i represents the index of the data point.

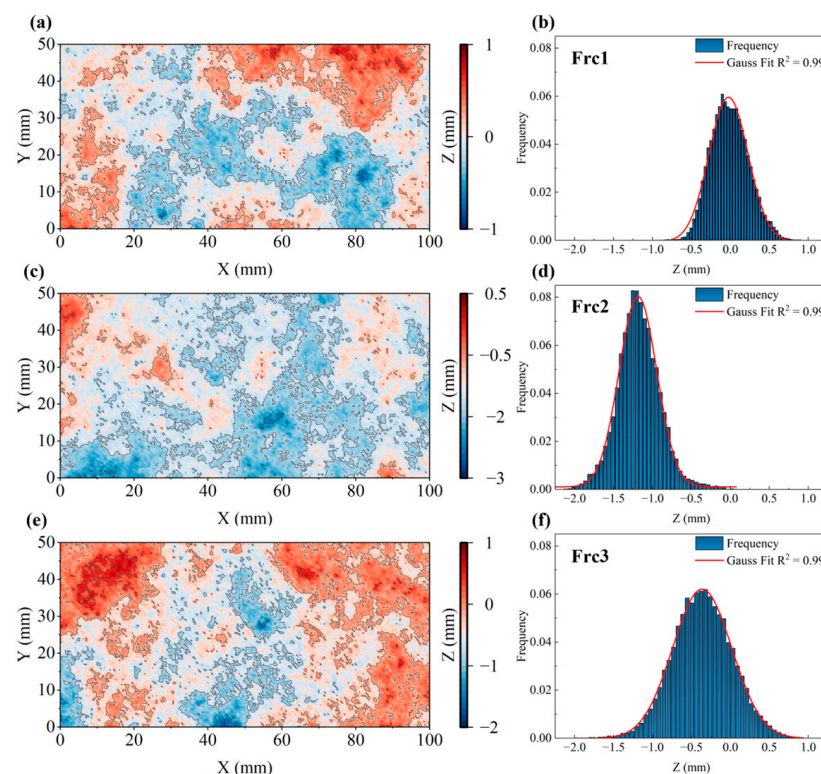


Figure 1. Morphology of fracture surfaces and corresponding surface-height distributions: (a,b) $JRC = 9.25$, (c,d) $JRC = 13.21$, and (e,f) $JRC = 17.15$.

It should be noted that Equation (3) is defined for a one-dimensional fracture profile, whereas the generated fracture surface in this study is two-dimensional. Therefore, the representative *JRC* of each fracture surface was not calculated from a single arbitrary profile. Instead, multiple longitudinal profiles parallel to the main flow direction were extracted from each generated fracture surface at equal spacing. The Z_2 value was first calculated for each profile using Equation (3), and the corresponding profile-based *JRC* was then obtained using Equation (4). The representative *JRC* of the fracture surface was finally determined as the arithmetic mean of these profile-based *JRC* values. This procedure reduces the dependence of the calculated *JRC* on a single transect and provides an averaged roughness descriptor for the two-dimensional fracture surface.

The calculated representative roughness values of the three fracture surfaces are 9.25, 13.21, and 17.15, respectively. To construct a geometric model suitable for three-dimensional solute transport simulations, each generated fracture surface was replicated and vertically translated, with the translation distance defined as the specified fracture aperture. In the present study, the upper and lower fracture walls were assumed to be perfectly mated, and the aperture was spatially uniform. This idealized setting was adopted to isolate the influence of wall roughness from shear-induced aperture heterogeneity, contact zones, and preferential flow channels. Following the vertical translation, Boolean operations were performed on the upper and lower fracture walls to seal the surrounding open regions, thereby forming the three-dimensional fracture model illustrated in Figure 2.

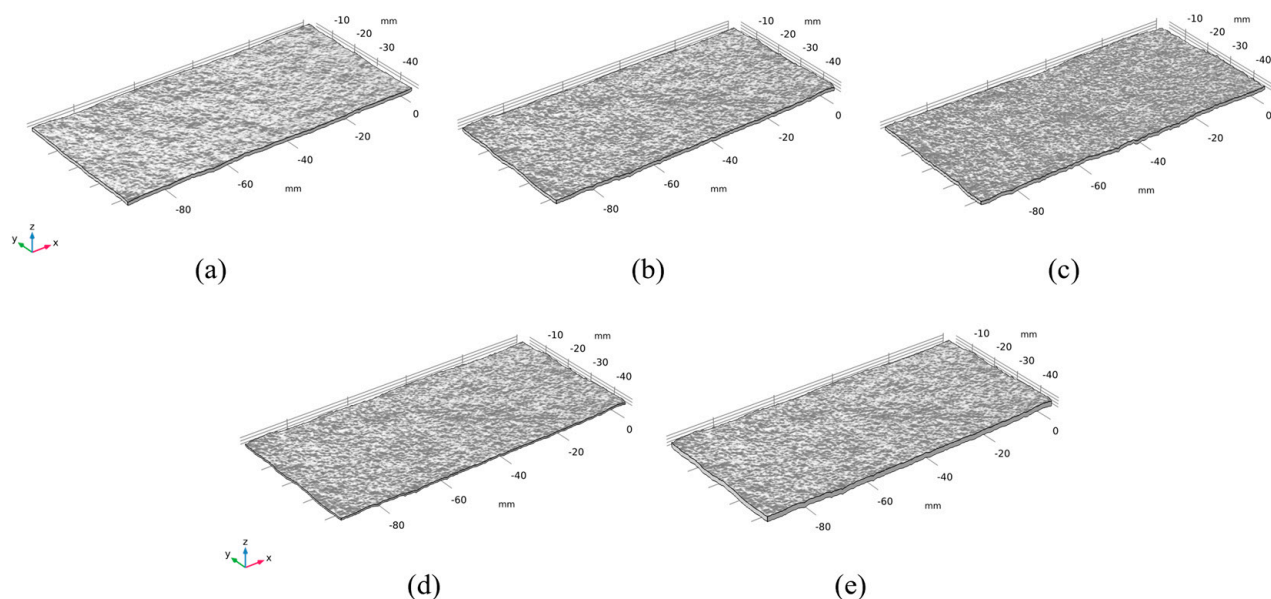


Figure 2. Three-dimensional fracture models used for numerical simulation: (a) *JRC* = 9.25; (b) *JRC* = 13.21; (c) *JRC* = 17.15; (d) *JRC* = 13.21; and (e) *JRC* = 17.15.

2.2. Governing Equations

The fluid flowing through the fracture model was assumed to be an isothermal, steady, incompressible Newtonian fluid. The seepage flow in the fracture was governed by the steady incompressible Navier–Stokes equations [47,48]:

$$\nabla \cdot \mathbf{u} = 0 \quad (5)$$

$$\rho \mathbf{u} \cdot \nabla \mathbf{u} = \mu \nabla^2 \mathbf{u} - \nabla P \quad (6)$$

where ∇^2 is the Laplace operator; $\mathbf{u}$ is the flow velocity vector; ρ is the fluid density; P is the pressure; and μ is the dynamic viscosity.

When the fluid within the fracture is at a low flow velocity or the velocity approaches zero, only molecular diffusion operates within the solution, and the solute transport process can be described by Fick's first law [49]:

$$J_d = -D_m \nabla C \quad (7)$$

where J_d is the diffusive flux, D_m is the molecular diffusion coefficient, and C is the volumetric concentration of the diffusing species.

Fick's first law describes diffusion driven by a concentration gradient. The solute diffuses from regions of high concentration to regions of low concentration, and the diffusive flux is proportional to the concentration gradient. For transient diffusion processes, where the solute concentration varies with time, Fick's second law can be expressed as [50]:

$$\frac{\partial C}{\partial t} = D_m \frac{\partial^2 C}{\partial x^2} \quad (8)$$

For the three-dimensional spatial coordinate system, the above equation can be further expressed as:

$$\frac{\partial C}{\partial t} = \nabla(D_m \nabla C) \quad (9)$$

Based on Fick's law, and applying the continuity principle and mass conservation theory, under the premise of neglecting solute molecule adsorption and mutual reactions, the advection–diffusion equation describing the coupling of advection and diffusion can be derived [20]:

$$\frac{\partial C}{\partial t} = -\nabla(uC) + \nabla(D_m \cdot \nabla C) \quad (10)$$

where $-\nabla(uC)$ represents the material transport process of the solute under the action of the flow velocity, and $\nabla(D_m \cdot \nabla C)$ represents the material diffusion process driven by the solute concentration difference.

2.3. Simulation Setup and Boundary Conditions

In the numerical simulations, water was used as the solvent under isothermal conditions at 25 °C. The density and dynamic viscosity of water were set to 999.0 kg/m³ and 8.90×10^{-4} Pa·s, respectively. Chloride ion (Cl[−]), a typical conservative solute in groundwater systems, was selected as the transported species. The molecular diffusion coefficient of Cl[−] in water was set to 2.03×10^{-9} m²/s.

The Péclet number Pe was used to characterize the relative importance of advective transport and molecular diffusion, and was calculated as follows:

$$Pe = \frac{Q}{WD_m} \quad (11)$$

where Q is the volumetric flow rate, W is the fracture width perpendicular to the flow direction, and D_m is the molecular diffusion coefficient. By varying the inlet velocity, a wide range of Pe values were obtained to investigate the transition of solute transport mechanisms under different hydrodynamic conditions. The simulated Pe values in the subsequent solute-transport analyses were $Pe = 0.1, 0.5, 1, 5, 10, 100, 1000$, and $10,000$.

Figure 3a shows the boundary conditions used in the numerical simulations. The fracture inlet was set as a velocity inlet, through which water entered the fracture at a prescribed constant velocity. The outlet was assigned an outflow boundary with a pressure of zero. The upper and lower fracture walls and the lateral boundaries were treated as impermeable no-flow boundaries. For solute transport, the solute was continuously injected from the inlet at a constant concentration, while the outlet was defined as an

open boundary with zero dispersive flux. The upper and lower walls and the lateral boundaries were assigned no-flux conditions, and solute adsorption and exchange at the fracture walls were neglected. Therefore, the present model describes conservative solute transport within an isolated fracture channel. Solute exchange with the surrounding rock matrix, matrix diffusion, adsorption, and chemical reactions were not considered in the present simulations.

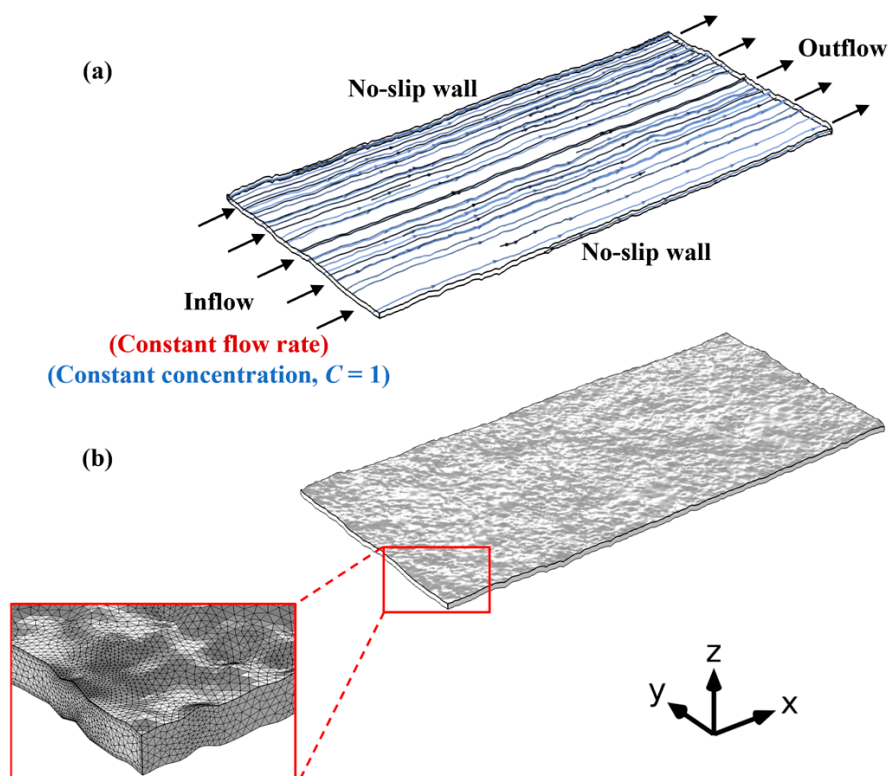


Figure 3. Boundary conditions and mesh model: (a) boundary conditions and (b) computational mesh.

As shown in Figure 3b, the fracture geometry was discretized using tetrahedral elements. To reduce potential mesh-size dependence, four mesh resolutions were tested using the reference fracture geometry, with element numbers of 224,257, 418,741, 998,603, and 2,847,060, corresponding to Coarse, Normal, Fine, and Extremely fine meshes, respectively. Under each mesh condition, solute transport was simulated at Pe values of 0.1, 1, 10, 100, 1000, and 10,000. Figure 4 presents the total solute flux and breakthrough curves obtained under different mesh resolutions. The results show that when the mesh resolution reached the Fine level or above, the total flux and breakthrough curves exhibited only minor differences, whereas the Coarse and Normal meshes produced more noticeable deviations. Therefore, the Fine mesh was adopted for all subsequent simulations to balance numerical accuracy and computational efficiency. The same mesh-generation strategy was applied consistently to the fracture models with different apertures and roughness levels. It should be noted that the mesh-independence verification was intended to confirm numerical stability for the representative fracture model used in this study, rather than to provide a complete mesh-sensitivity analysis for all possible roughness and aperture combinations. For fractures with stronger geometric heterogeneity, shear-induced contact zones, or highly localized vortical structures, additional local mesh refinement may be required in future studies.

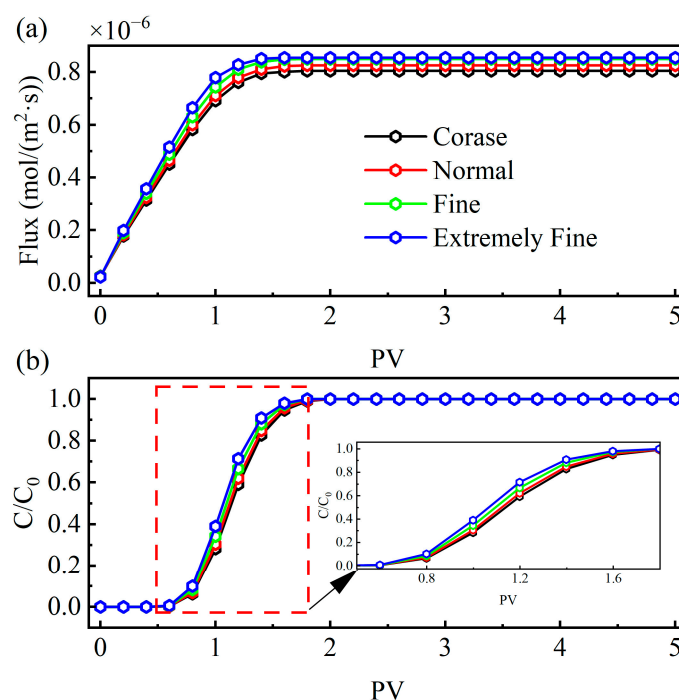


Figure 4. Mesh-independence verification: (a) total solute flux curves and (b) solute breakthrough curves under different mesh resolutions.

3. Results

3.1. Fluid Flow Behaviour in Fractures

Figure 5 shows the evolution of the vorticity field in fracture Frc2 with an aperture of 1 mm under different Pe conditions. When Pe is lower than 1000, the vorticity magnitude remains very low throughout the fracture, indicating that the flow field is mainly characterized by stable laminar flow and that local vortices have a limited influence on the overall flow structure. As Pe increases to 1000 and above, the vorticity magnitude increases markedly, and localized high-vorticity regions begin to appear near the rough fracture walls. This change indicates that increasing inlet velocity enhances inertial effects and promotes local flow instability within the rough fracture. As the Reynolds number increases from 2.03 to 20.3, the flow field gradually shifts from a nearly uniform laminar state to a more heterogeneous state affected by local vortical structures.

Figure 6 presents the streamline distributions under different fracture geometric conditions. With increasing fracture aperture, the available flow space expands, and the streamlines become more uniform and less constrained by the wall geometry. This indicates that a larger aperture can weaken the relative influence of wall roughness on the main flow path and promote smoother fluid migration through the fracture. In contrast, increasing surface roughness enhances the tortuosity of streamlines and causes local deviations in the flow direction. However, because the upper and lower fracture surfaces are perfectly mated in the present models, the roughness effect is mainly reflected in local streamline bending rather than in the formation of strong preferential flow channels. Therefore, aperture primarily controls the overall flow capacity, whereas roughness mainly modifies the local flow-path tortuosity. This behavior is closely related to the idealized fracture geometry adopted in this study, in which the upper and lower fracture surfaces are perfectly mated and the aperture is spatially uniform. Under this condition, roughness mainly induces local streamline bending rather than strong three-dimensional channeling caused by aperture heterogeneity or contact zones.

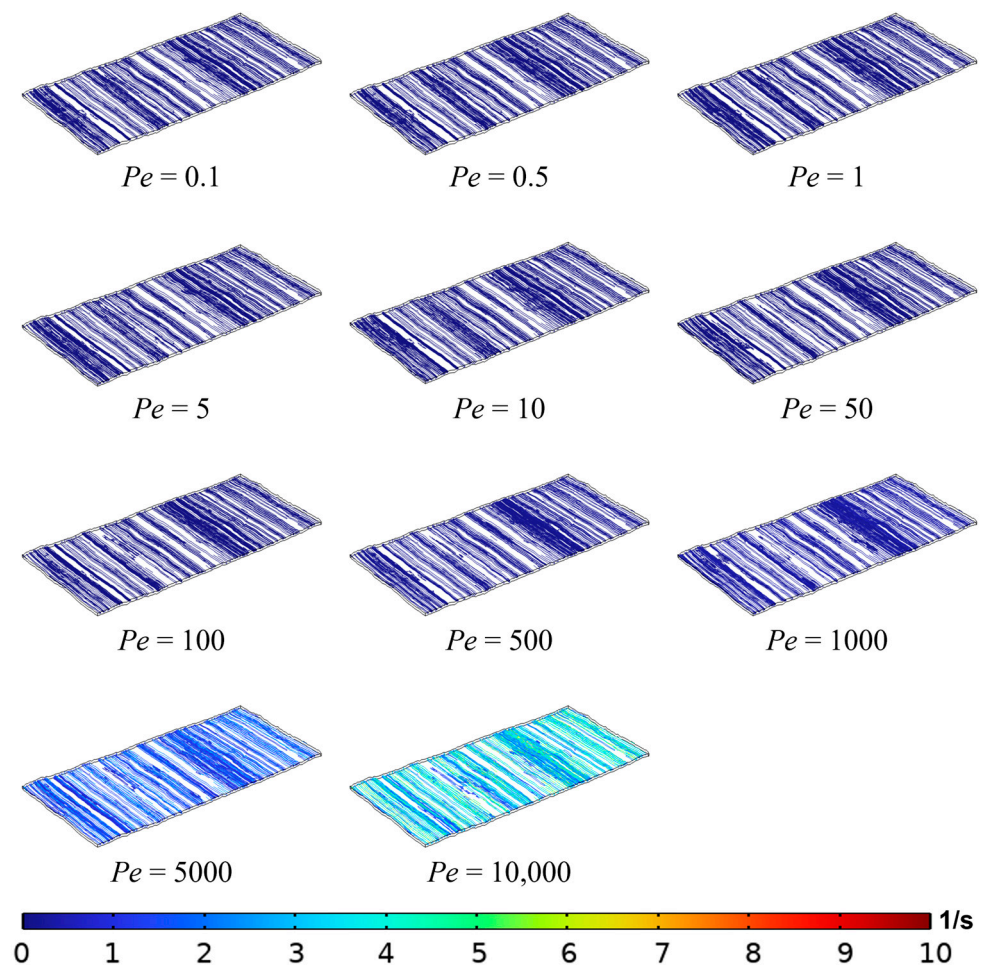


Figure 5. Evolution of the vorticity field in Frc2 ($e = 1$ mm) under different Pe conditions.

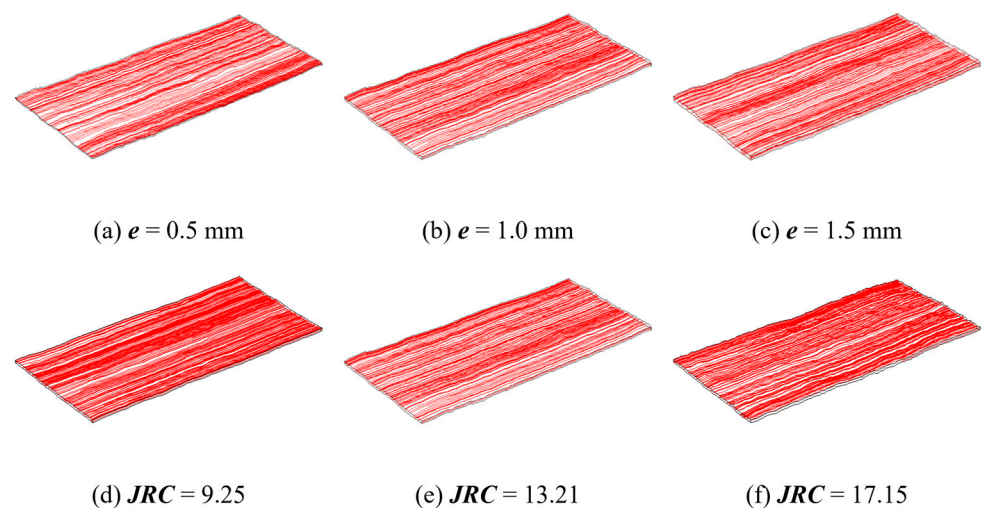


Figure 6. Streamline distributions in fractures under different geometric constraints.

3.2. Evolution of the Concentration Fields in Fractures

To intuitively illustrate the solute transport behavior within fractures under different hydrodynamic conditions, Figure 7 presents the solute concentration field distributions in Frc2 under varying Pe conditions. The results demonstrate that as the Pe gradually increases, the solute transport behavior within the fracture is significantly affected, with the concentration field distribution exhibiting distinct variations. With increasing Pe , the solute

transport mechanism within the fracture exhibits three characteristic regimes. In the low- Pe regime ($Pe \leq 0.1$), molecular diffusion dominates, and the concentration field tends to become relatively homogenized without a distinct transport front. The case of $Pe = 0.5$ represents a transitional state between diffusion-dominated and macro-dispersion-dominated transport. In the intermediate- Pe regime ($0.1 < Pe < 1000$), advection and diffusion interact, and the transport behavior is mainly characterized by macro-dispersion, with a clear concentration-gradient transition zone. In the high- Pe regime ($Pe \geq 1000$), transport becomes strongly advection-controlled and exhibits Taylor-dispersion-like characteristics. Under this condition, the solute front becomes sharper, and the gradual transition zone is substantially narrowed.

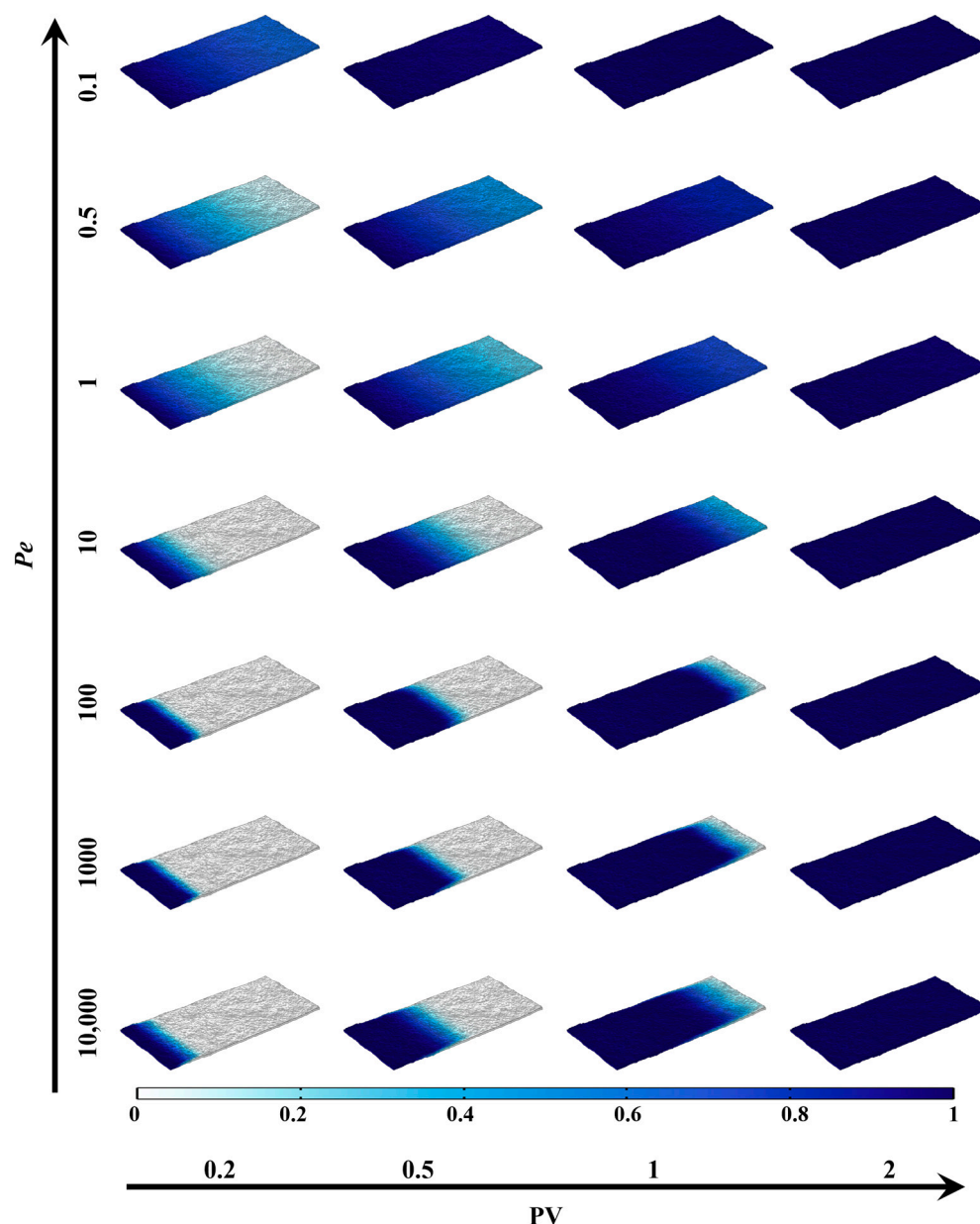


Figure 7. Solute concentration fields in Frc2 under different Pe conditions and injected pore volumes (PVs).

Figure 8 presents the distribution characteristics of the solute concentration field in Frc2 under varying aperture conditions ($PV = 0.2$). As can be observed, the increase in aperture further promotes molecular diffusion behavior within the fracture. At an aperture

of 0.5 mm, the concentration field distribution within the fracture gradually transitions from a molecular diffusion pattern to a sharp front pattern with increasing Pe . With increasing aperture, the extent of solute diffusion under conditions with $Pe < 10$ exhibits a significant increase, while under conditions with $Pe \geq 10$, the extent of the transition zone at the solute front also increases. These results indicate that increasing aperture promotes solute spreading and broadens the concentration transition zone, especially under low-to-intermediate Pe conditions.

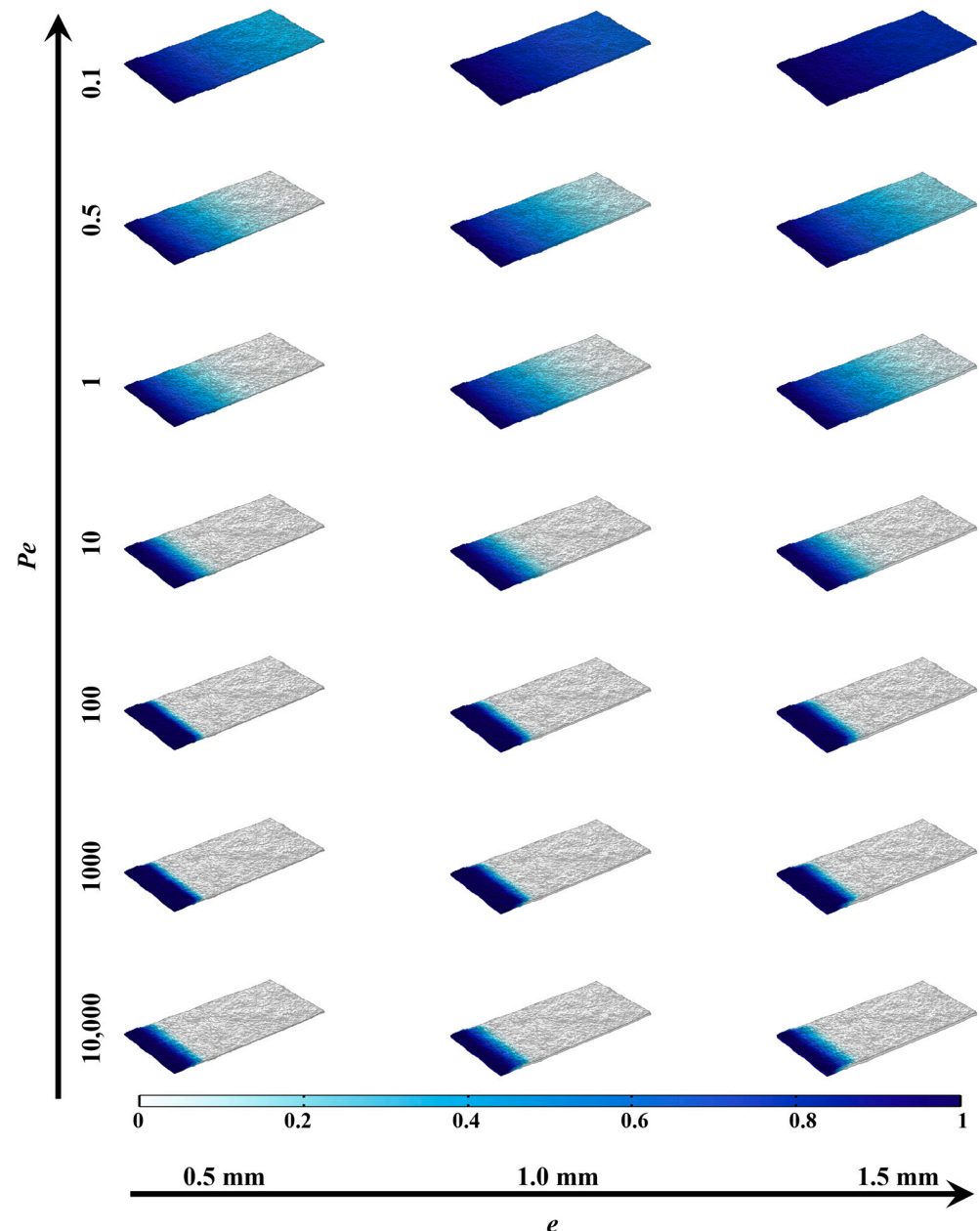


Figure 8. Solute concentration fields in Frc2 under different apertures (e) and Pe values at $PV = 0.2$.

Figure 9 further compares the concentration-field distributions under different roughness conditions. Unlike the aperture effect, increasing JRC does not substantially change the overall concentration-field pattern under the idealized fracture geometries considered in this study. The primary influence of roughness is reflected in the local bending and tortuosity of the concentration front, while the macroscopic migration pattern remains broadly similar among the three roughness levels. This behavior is related to the geometric

assumption adopted here: the upper and lower fracture surfaces are perfectly mated, and the aperture is spatially uniform. Under this condition, roughness mainly changes the local flow-path geometry but does not generate significant aperture heterogeneity, contact zones, or preferential flow channels. Therefore, the limited influence of roughness observed in this study should be interpreted as conditional on the present perfectly mated and uniform-aperture fracture models, rather than as a general conclusion for all natural rough fractures.

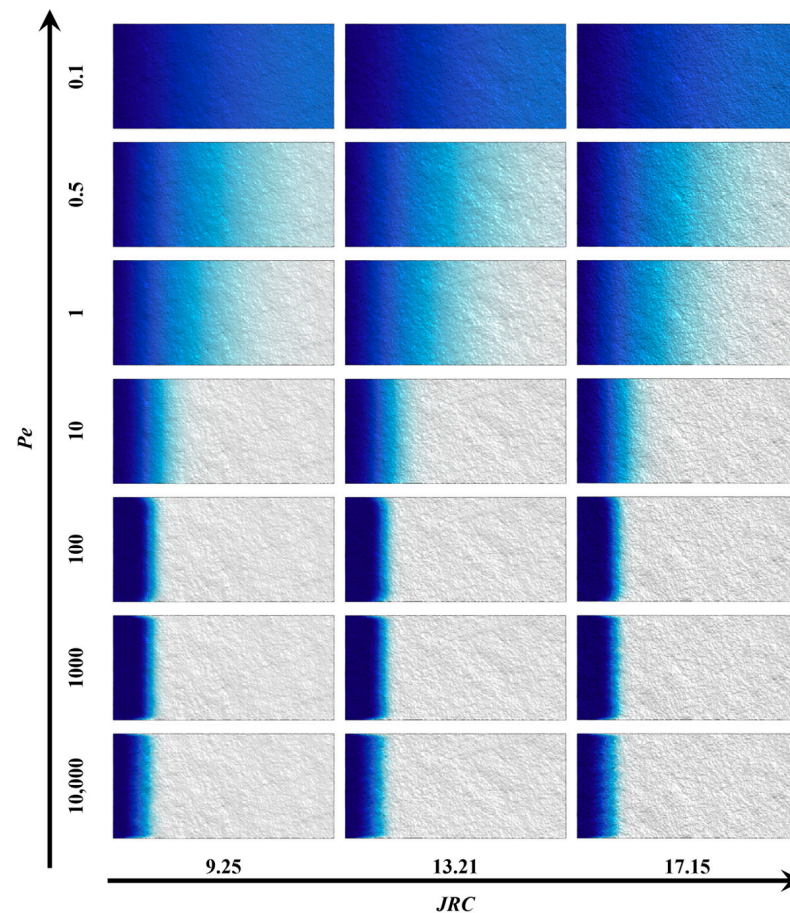


Figure 9. Solute concentration fields under different roughness (*JRC*) conditions and *Pe* values at *PV* = 0.2.

Figure 9 illustrates the distribution characteristics of the solute concentration field within fractures under different roughness conditions. As can be seen, compared with the variations in the solute concentration field under different aperture conditions, the increase in roughness does not produce a significant effect on the concentration field distribution, only inducing a localized increase in the tortuosity of the concentration front. This phenomenon is similar to that observed by Wang et al. [5] in non-dislocated fractures with varying roughness. This is attributable to the fact that the fracture models employed in this study are all models with perfectly mated upper and lower fracture surfaces and uniform aperture, where the solute transport behavior is influenced solely by the tortuosity characteristics of the fracture walls. This contrasts with the phenomena observed in studies employing fracture models with heterogeneous aperture distributions [21], where local aperture variations are more prone to forming preferential flow paths, thereby altering the morphological characteristics of the solute transport front.

3.3. Evolution of the Solute Breakthrough Curves

To further analyze the solute breakthrough behavior during the transport process, the average concentration of the solute flowing through the fracture outlet was normalized. Figure 10 presents the solute breakthrough curves in Frc2 under different aperture conditions. As can be observed, with increasing Pe , the evolution trend of the solute breakthrough curves within the fracture exhibits staged variations. As shown in Figure 10a,b,c, at a Pe of 0.1, the solute breakthrough curve exhibits a trend in which the slope gradually decreases to zero with increasing PV. As the Pe increases to 1, the slope of the curve gradually decreases and the rate of increase slows, ultimately approaching zero. With a further increase in the Pe , the solute breakthrough curve exhibits a stagnation period in the initial stage, during which the curve does not increase significantly; after reaching a certain PV, it rises rapidly to near the maximum value of the curve and then tends toward a constant value. The above phenomena indicate that at a Pe of 0.1, molecular diffusion dominates within the fracture, and the molecular diffusion behavior is not significantly affected by the flow velocity effect. A pronounced early arrival phenomenon occurs, allowing the solute to diffuse to the fracture outlet under relatively low PV conditions. As the Pe increases, the influence of advection intensifies, and molecular diffusion is suppressed, thereby reducing the solute breakthrough efficiency in the initial stage. When the Pe further increases to 5 and above, the molecular diffusion behavior within the fracture is further suppressed. With increasing Pe , the solute breakthrough curve increasingly exhibits characteristics more akin to a step function, at which point the solute transport behavior within the fracture is dominated by advection, and the time for complete solute breakthrough approaches the time required for the injected fluid to reach the outlet.

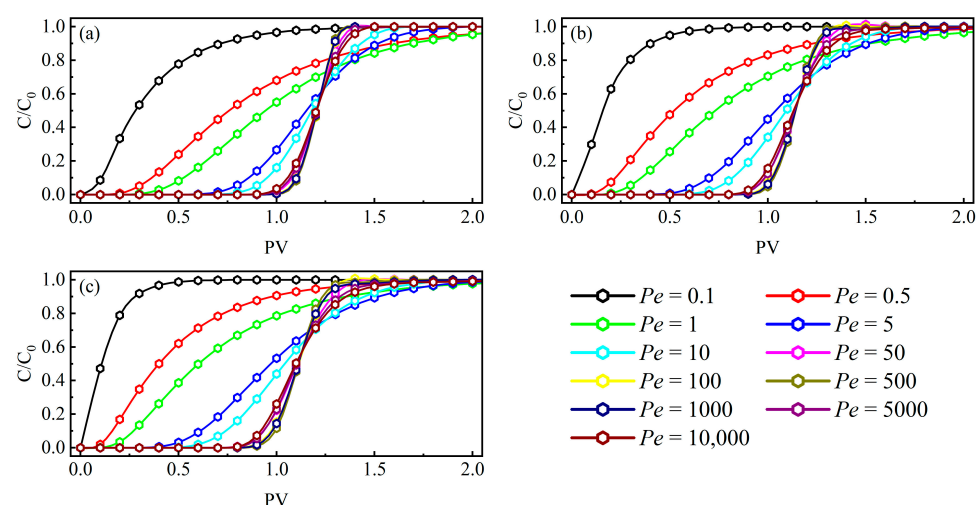


Figure 10. Solute breakthrough curves (BTCs) in Frc2 under different apertures: (a) $e = 0.5$ mm, (b) $e = 1.0$ mm, and (c) $e = 1.5$ mm.

Figure 11 illustrates the evolution of the outlet solute concentration as a function of Pe and fracture aperture at selected pore volumes ($PV = 0.2, 0.5$, and 1.0). As Pe increases, the solute transport mechanism gradually shifts from diffusion-dominated spreading to non-equilibrium advection-controlled transport. At $PV = 0.2$ and $PV = 0.5$, the normalized outlet concentration decreases rapidly from near unity to nearly zero with increasing Pe , reflecting the suppression of early diffusion-driven breakthrough under higher Pe conditions. In contrast, under relatively high- Pe conditions, the solute cannot readily diffuse throughout the fracture before advective breakthrough occurs; therefore, the early breakthrough observed under low- Pe conditions becomes progressively weakened.

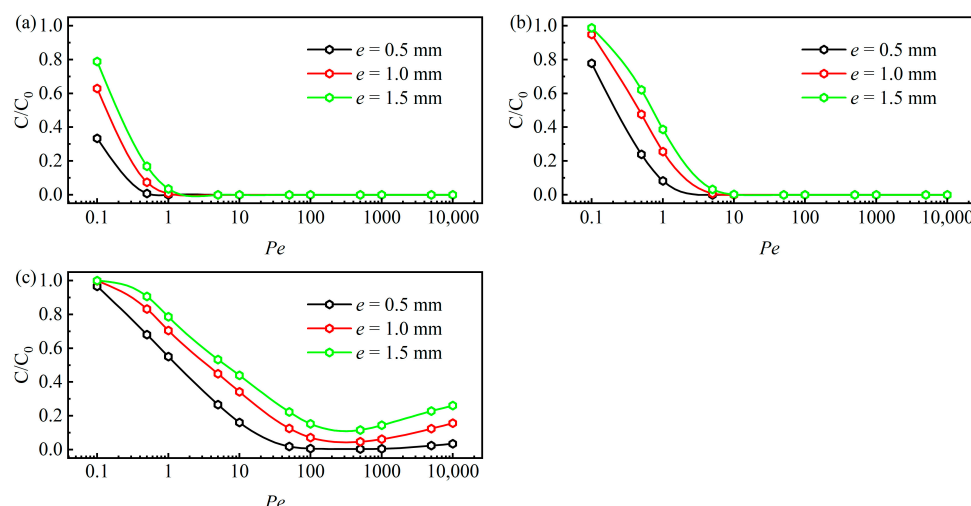


Figure 11. Normalized outlet concentrations at selected pore volumes: (a) $PV = 0.2$, (b) $PV = 0.5$, and (c) $PV = 1.0$ in Frc2 under different aperture conditions.

Figure 12 presents the solute breakthrough curves under different roughness conditions. The BTCs of fractures with different JRC values exhibit similar overall trends with increasing Pe , transitioning from an early breakthrough type under low Pe conditions to step-like breakthrough behavior under high- Pe conditions. The concentration values extracted at different PVs in Figure 13 also show limited differences among the three roughness levels. Combined with the concentration-field distributions shown in Figure 9, these results indicate that, for the perfectly mated and uniform-aperture fracture models considered here, JRC mainly affects local front tortuosity and has a limited influence on the overall outlet breakthrough behavior. However, this result should not be generalized to natural fractures with shear displacement, partial mismatch, contact areas, or heterogeneous aperture distributions. In such fractures, roughness may significantly influence solute transport by modifying aperture connectivity, local velocity distributions, stagnant zones, and preferential pathways.

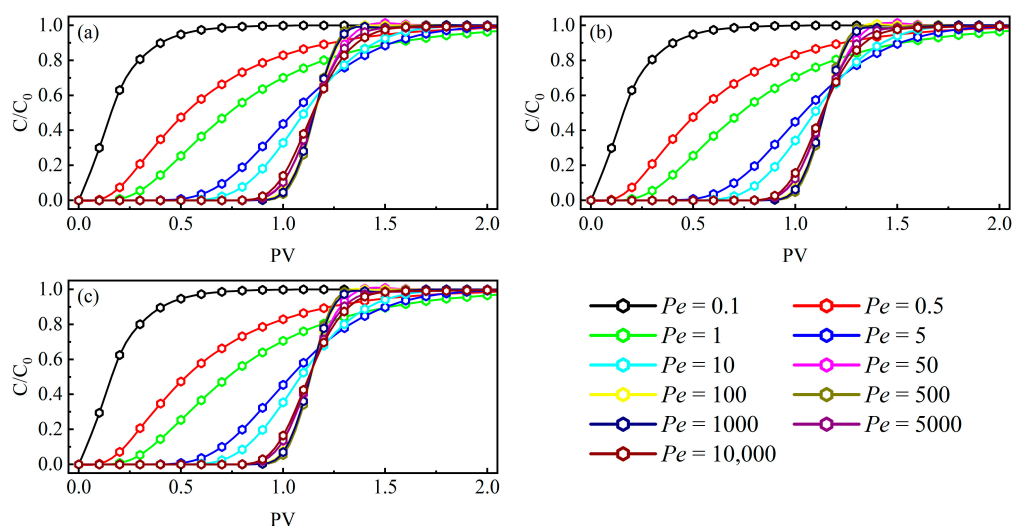


Figure 12. Solute breakthrough curves (BTCs) in fractures under different roughness conditions: (a) $JRC = 9.25$, (b) $JRC = 13.21$, and (c) $JRC = 17.15$.

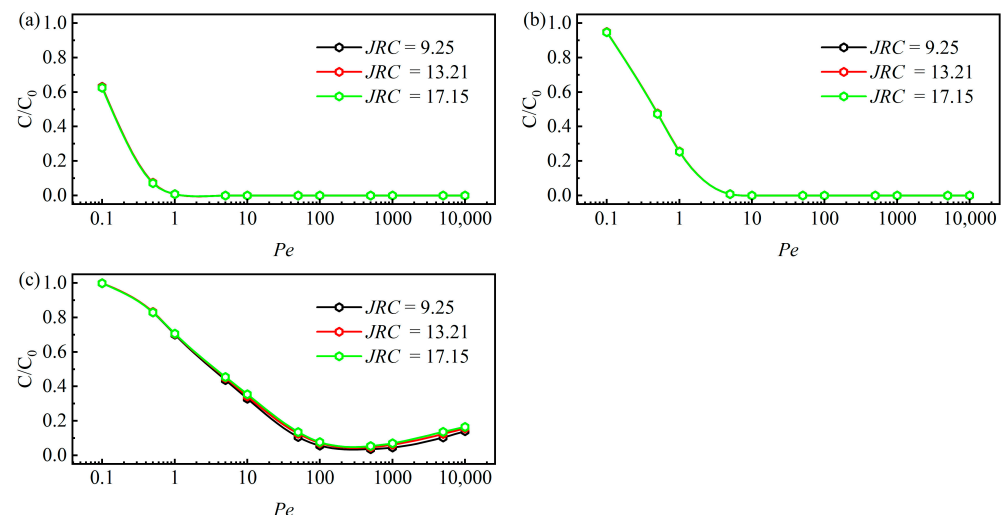


Figure 13. Normalized outlet concentrations at selected pore volumes: (a) $PV = 0.2$, (b) $PV = 0.5$, and (c) $PV = 1.0$ under different roughness conditions.

4. Discussion

4.1. The Effect of Hydrodynamic Conditions on Dispersion Mechanisms

Figure 14 systematically reveals the evolution of solute flux and the transition of dominant physical mechanisms in fractured media under hydrodynamic conditions represented by different Péclet numbers (Pe), exhibiting an overall pronounced transitional characteristic from molecular diffusion dominance at low Pe to advection and Taylor dispersion dominance at high Pe . Drawing upon the relevant studies of numerous researchers, the solute dispersion mechanisms can be further classified as follows: molecular diffusion dominates at relatively low Pe levels ($10^{-3} < Pe < 10^{-1}$), followed by macro-dispersion dominance at intermediate levels ($10^{-1} < Pe < 10^3$), and finally Taylor dispersion dominance at high levels ($Pe > 10^3$) [14,21,23].

As the Pe varies from low to high, the solute transport mechanism undergoes a continuous evolution from molecular diffusion to macro-dispersion to Taylor dispersion, with the corresponding diffusive flux and advective flux curves exhibiting distinct interval-specific differences. Specifically, as shown in Figure 14a,b: in the low Pe regime (e.g., $Pe = 0.1$), the solute flux in the early stage is primarily contributed by the diffusive flux, which exhibits a pronounced peak during the initial stage of fluid injection ($PV < 0.5$) and subsequently decays rapidly, whereas the advective flux shows a slow growth trend, indicating that molecular diffusion is the controlling transport mechanism at this stage. As the Pe increases to the intermediate-to-high range, the advective flux gradually becomes dominant, with its magnitude significantly elevated compared with the diffusive flux at low Pe , and it rapidly reaches a steady value between $PV = 1$ and 2 (as shown in Figure 14c). Concurrently, the contribution of the diffusive flux approaches zero (as shown in Figure 14b), revealing that advection has completely superseded diffusion and become the absolute driving force for fluid and solute migration.

Based on the above patterns, Figure 14d further summarizes and proposes three typical flux behavior modes: Type 1 corresponds to the molecular diffusion-dominated regime ($Pe < 0.1$), where the flux curve is characterized by a significant and relatively steady diffusive flux, with the maximum contribution of the advective flux remaining lower than that of the diffusive flux; Type 2 corresponds to the transitional mixed regime of macro-dispersion and diffusion ($0.1 < Pe < 1000$), where diffusion still exerts a certain influence on the solute transport process, and with continuous fluid injection, the advective flux rapidly escalates and surpasses the initial diffusive flux to become dominant; and Type

3 corresponds to the strong advection and Taylor dispersion-dominated regime ($Pe > 1000$), exhibiting typical step-like and plateau characteristics, where the diffusive flux is virtually negligible and the advective flux remains in an absolutely dominant position throughout. A comprehensive analysis of this series reveals that under low- Pe conditions, the early breakthrough and retention effects caused by diffusion must be fully considered, whereas under high- Pe conditions, the prediction of the principal flux peak can be focused on advection-dominated transport models. This provides a targeted theoretical basis for the simulation and prediction of solute transport in fractured media.

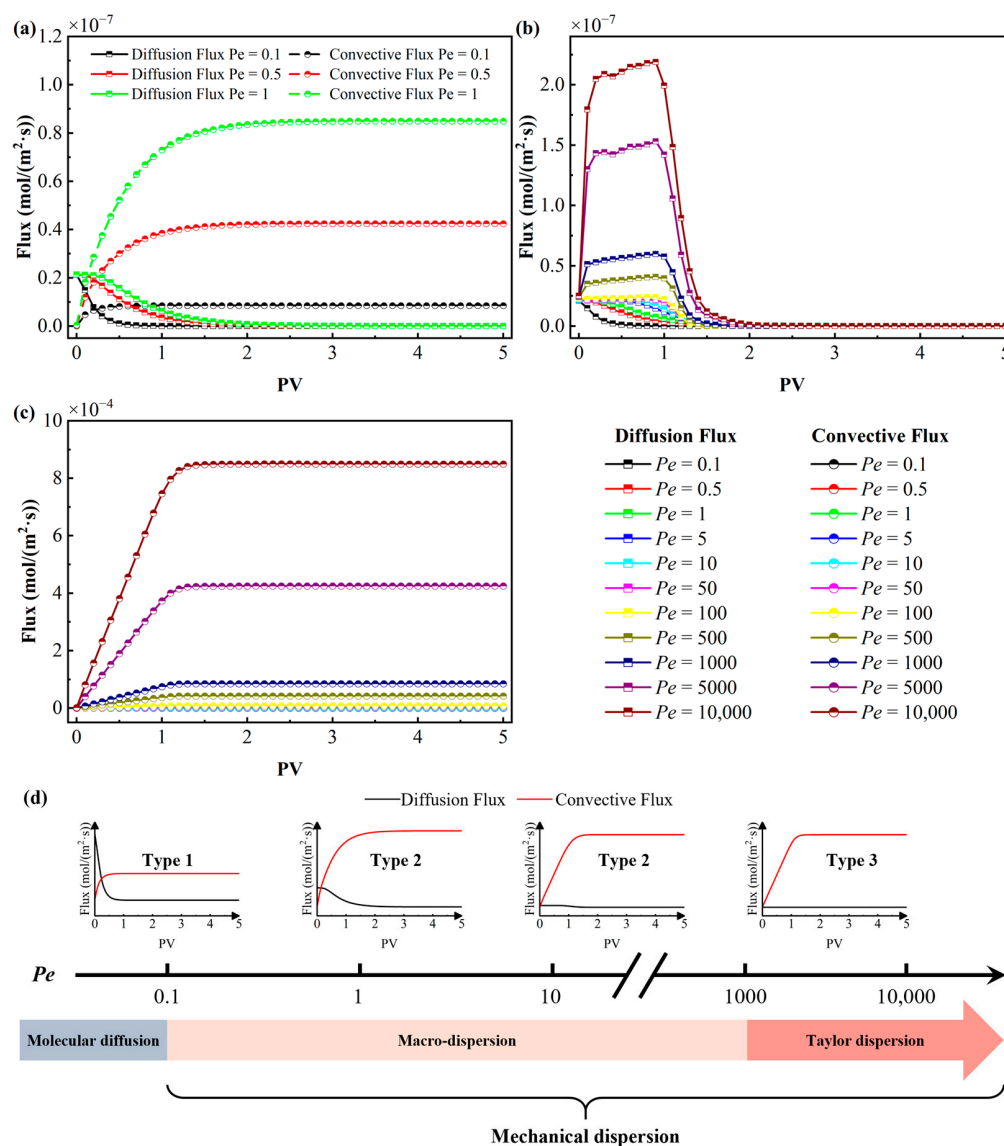


Figure 14. Solute flux curves in fracture Frc2 under different hydrodynamic conditions (Pe): (a) Diffusion flux and convective flux curves in Frc2 for Pe values of 0.1, 0.5, and 1; (b) Diffusion flux curves in Frc2 under different Pe conditions; (c) Convective flux curves in Frc2 under different Pe conditions; (d) Typical flux curves under different diffusion mechanisms.

However, the above interpretation should be understood within the assumptions of the present numerical model. The fracture models used in this study have perfectly mated upper and lower walls and spatially uniform apertures. Solute exchanges with the surrounding rock matrix, matrix diffusion, adsorption, and chemical reactions were not considered. In addition, mesh-independence verification confirms numerical stability, but it does not fully replace validation against analytical solutions or laboratory experiments.

Therefore, the Pe -controlled transport regimes identified here should be interpreted as numerical observations under the specific assumptions of the present idealized fracture-channel model.

4.2. Fracture-Scale Implications for Groundwater Contamination Assessment

The Pe -controlled transition of solute transport mechanisms has implications for groundwater contamination assessment in fractured media. Under low- Pe conditions, molecular diffusion may cause early solute spreading even when the mean flow velocity is low. This indicates that contaminants may spread within connected fracture spaces under weak-flow or nearly stagnant conditions if a persistent concentration gradient exists. Therefore, in low- Pe environments, attention should be paid not only to advective migration pathways but also to diffusion-driven spreading and early contamination signals.

Under intermediate- Pe conditions, diffusion and advection coexist, and the solute transport behavior is controlled by a mixed mechanism. In this regime, the contaminant front may be broadened by diffusion and local velocity variations, while advective transport gradually becomes increasingly important. Therefore, monitoring and remediation strategies should consider both the early spreading behavior and the subsequent advective migration process. A hybrid monitoring strategy may be more appropriate than a single advection-based prediction approach.

Under high- Pe conditions, solute migration is mainly controlled by advection, and the concentration front becomes sharper. This implies that contaminants may migrate rapidly along the main flow direction and may arrive at downstream locations abruptly after a relatively short transition period. For such conditions, monitoring wells and remediation barriers should be arranged with particular attention to the main advective flow paths and possible preferential channels.

Nevertheless, the practical implications of this study should be interpreted cautiously. The present model describes conservative solute transport within an isolated fracture channel and does not include matrix diffusion, adsorption, chemical reactions, or fracture–matrix exchange. In real fractured aquifers, matrix diffusion may cause contaminant retention and long-term tailing, especially under low- Pe conditions. Shear displacement, partial mismatch between fracture walls, contact zones, and heterogeneous aperture distributions may also generate preferential flow paths and stagnant zones, thereby altering the breakthrough behavior. Therefore, the findings of this study provide fracture-scale insights into Pe -controlled transport regimes under idealized assumptions, rather than a complete prediction framework for natural fractured aquifers.

Future studies should further consider fracture–matrix coupled transport, dual-porosity models, matrix diffusion, reactive transport, stochastic rough-fracture realizations, and shear-induced aperture heterogeneity. Benchmark simulations using smooth parallel-plate fractures and comparisons with analytical solutions or laboratory tracer experiments would also be useful for further validating the numerical model and evaluating the generality of the Pe -controlled transport regimes identified in this study.

5. Conclusions

This study investigated Pe -controlled conservative solute transport in idealized rough rock fractures with perfectly mated walls and spatially uniform apertures. By jointly analyzing concentration-field evolution, breakthrough curves, and diffusive/advective fluxes, the transport-regime transition over a wide range of Pe values was examined. The main conclusions are as follows:

- (1) With increasing Pe , solute transport in the idealized rough fracture exhibits a staged transition from diffusion-dominated transport to mixed macro-dispersion-dominated

transport and finally to high-Pe advection-controlled transport with Taylor-dispersion-like characteristics. Under low-Pe conditions, molecular diffusion controls early solute spreading and may lead to early breakthrough. Under intermediate-Pe conditions, diffusion and advection interact, forming a broadened concentration transition zone. Under high-Pe conditions, advection becomes dominant, the solute front becomes sharper, and the BTCs gradually approach step-like breakthrough behavior.

- (2) Fracture aperture has a stronger influence on solute spreading than wall roughness under the geometric assumptions considered in this study. Increasing aperture enhances solute spreading and broadens the concentration transition zone, especially under low-to-intermediate Pe conditions. In contrast, for the perfectly mated and uniform-aperture fracture models considered here, increasing JRC mainly induces local tortuosity and bending of the concentration front, while its influence on the overall outlet BTCs is limited. This conclusion should not be generalized to natural fractures with shear displacement, partial wall mismatch, contact zones, or heterogeneous aperture distributions, where roughness may significantly affect solute transport by modifying aperture connectivity, stagnant zones, local velocity distributions, and preferential flow paths.
- (3) Flux decomposition further confirms the Pe-controlled transition of transport mechanisms. In the low-Pe regime, diffusive flux contributes significantly to early solute spreading. In the intermediate-Pe regime, advective flux increases rapidly and gradually becomes dominant while diffusion still contributes to solute-front broadening. In the high-Pe regime, advective flux dominates the overall transport process, whereas diffusive flux becomes relatively small. Therefore, the combined analysis of concentration fields, BTCs, and flux components provides a more complete interpretation of Pe-controlled transport regimes than using BTCs alone.
- (4) The results provide fracture-scale insights for classified groundwater contamination risk assessment under conservative transport assumptions. Low-Pe systems require attention to diffusion-driven spreading and early breakthrough, intermediate-Pe systems require consideration of mixed diffusion–advection transport, and high-Pe systems require monitoring of rapid advection-controlled migration. However, the implications should be interpreted within the assumptions of the present model, including perfectly mated fracture walls, uniform aperture, conservative solute transport, no matrix diffusion, no adsorption, and no chemical reactions.
- (5) This study still has several limitations. The model does not consider solute exchange with the surrounding rock matrix, matrix diffusion, adsorption, reactive transport, shear-induced aperture heterogeneity, or contact-zone evolution. In addition, although mesh independence was verified, no smooth parallel-plate benchmark or laboratory tracer validation was included. Future studies should incorporate fracture–matrix coupled models, dual-porosity transport, stochastic rough-fracture realizations, high-roughness mesh verification, smooth-fracture benchmark tests, and experimental validation to further evaluate the generality of the Pe-controlled transport regimes identified in this study.

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