Shear enhanced nonlinear flow in rough-walled rock fractures

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Highlights:

- Channeling and eddy flow behaviors in 3D rough-walled rock fractures enhanced by shear created asperity contacts;
- Nonlinear relationship between flowrates and pressure gradients in the 3D fractures;
- Nondeterministic relationship between effective transmissivity and local apertures;
- Limitations of simplified 2D models in modeling nonlinear flow behaviors in rough-walled fractures.

Abstract: Nonlinear flow in 3D rough-walled rock fracture models are simulated by solving the Navier-Stokes equations in this paper. The emphasis is on the impacts of shear caused aperture changes (variable apertures and asperity contacts) and flow conditions (inertial term) upon nonlinear flow behaviors in 3D rough-walled rock fractures. In order to compare shear effects, two 3D fracture models, with and without shear process, were established with the identical initial rough-walled surfaces tomography of a realistic rock sample. Five groups of simulations with different inflow boundary conditions of flowrates/Reynolds numbers (Re) were conducted to demonstrate shear enhanced nonlinearity of flow fields and limitations of local cubic law (LCL) approach. The flow results clearly show channeling flow along the preferential fluid paths, transverse flow around the contact spots and eddy flows behind contact spots with increasing Re numbers, which cannot be observed in 2D models. The effective transmissivity of the 3D fracture model was calculated from the modeling results of velocity and pressure fields. The results showed that the effective transmissivity is a function of local apertures with important uncertainties even when Re is small (i.e. $Re = 0.4$ in this study), thus the validity of the transmissivity evaluation using LCL approach for nonlinear flow in 3D rough-walled rock fractures is questionable. The mechanical effects, i.e. stress and shear caused aperture space changes and asperity contacts should be considered for modeling flow and mass/energy transport processes in rough-walled fractures in 3D.

Keywords: rough-walled rock fractures; shear; contact spots; nonlinear fracture flow; eddy flow; effective transmissivity.

1 Introduction

Modeling of fluid flow and characterization of hydraulic transmissivity of single rock fractures plays a critical role in understanding fluid flow behaviors in rock masses with complex fracture networks, which is of great importance for many environmental issues and rock engineering problems [1-2].

The early and simple approach to describe the flow in single rock fractures is the well-known cubic law (CL). This approach is based on the smooth parallel plate assumption, which simplified the flow process both in geometry and physics by ignoring the surface roughness and inertial/nonlinear aspects of fluid flow in rough fractures. When the surface roughness needs to be considered, the CL model was assumed to be locally applicable (LCL). In this case the aperture space is discretized with meshes based on the scanned surface topography data. Due to its simplicity and ability to model effects of surface roughness, the LCL model have been widely applied for modeling flow in rock fractures [1, 3-5].

Many modified LCL models and corrected local effective transmissivity models were developed to improve the inadequate representation of geometry conditions with the traditional LCL approach. This was undertaken by considering local roughness parameters and/or weak inertial impacts of flow. Ge [6] proposed a modified model considering the tortuosity of flows in rough fractures. Oron and Berkowitz [7] reexamined critical assumptions of LCL and analytically discussed the importance of local geometry, tortuosity and contact effects. Wang et al. [8] developed a modified LCL model to consider impacts of tortuosity, local roughness and weak inertial terms through an empirical correction factor, C , obtained from numerical investigations on 2D symmetric wedges.

The fundamental understanding of flow and transport behavior in rough-walled rock fractures cannot be adequately represented by using simplified CL and LCL approaches, since the combined effects of the complex surface roughness and inertial/nonlinear terms cannot be fully considered by them. This led to a series of researches from theoretical analysis [e.g., 7-10], experimental investigations [e.g., 11-19] and numerical studies [e.g., 20-24]. Meanwhile, to consider complicated flow conditions, nonlinear models for the relationship between flowrates and pressure gradients, such as Forchheimer's law, have also been widely applied to describe the nonlinear flow behaviors observed in both laboratory experiments and numerical simulations [15-16, 19]. More importantly, the mechanical effects on fractures, including normal compression and shear dilation, significantly change the aperture space and form contact spots, which is an important issue affecting flow and transport behavior in rough-walled rock fractures [26-33].

Due to the difficulty in monitoring evolutions of aperture and contact spots during mechanical loading processes, the mechanical impacts on nonlinear flow in natural 3D fractures have not been investigated in adequate details in laboratory tests. Therefore, a few integrated laboratory tests and numerical studies by solving the 3D Navier-Stokes equations (NSE) for modeling flow in rough-walled rock fractures have been published. The first integrated laboratory experiments by testing fluid flow in a replica sample of natural fracture and numerical modeling by solving the NSE in 3D for fluid flow in rock fractures was reported in Refs. [12] and [13]. It was found that weak inertia regimes exist when Reynolds numbers (Re) in the range of 1.0 to 10.0 for the fracture models used, where the normalized hydraulic transmissivity nonlinearly decreasing with increasing Re values. Crandall et al. [34] simulated fluid flow in a series of 3D models of rough-walled fractures by solving NSE in 3D and found that the transmissivity decreased with the increase of the surface fractal dimensions. Xiong et al. [35] reported integrated laboratory experiments and 3D numerical modeling results of flow in rough-walled rock fractures, which considered the impacts of shear displacement on the transmissivity of fractures. Quantitative observations and presentations of the eddy flow regions in rock fractures were recently reported in Refs. [17] and [18] through integrated laboratory testing and numerical modeling. Wang et al. [8] recently implemented numerical simulations of flow with local Re around 0.02 in rough-walled fractures, by solving NSE in 3D and proposed a modified LCL through an empirical correction factor. These studies generally illustrated the impacts of surface roughness and weak inertial effects on the flow behaviors in rock fractures in 3D. However, the impacts of variable aperture space and contact spots due to shear, as well as strong inertial effects on the nonlinear flow behaviors, remain largely unstudied in adequate details for understanding the realistic flow behaviors as well as the effects of channeling, transverse and eddy flow features. Therefore, the detailed complexities of nonlinear flow fields by numerical solution of NSE in 3D, with or without mechanical effects of compression and shear mechanisms included, have not been well presented, described and analyzed.

It should be noted that most of the published modified models considered only much simplified fracture surface topography, parameters or specific flow conditions (e.g. low Re values for insignificant nonlinearity). Detailed flow velocity fields were rarely presented in most of the publications, which made adequate understanding of the causes of flow complicity by roughness impossible. Therefore, realistic complicity of the nonlinear flow fields in proper details, caused by both mechanical loading and strong inertial effects, and the limitations of the LCL approach for natural 3D rough-walled fractures still remain as open

questions. In addition, simplified 2D models formed by cutting through cross-sections of real fractures have been widely used to model fracture flows [e.g. 20-25, 30]. However, these simplified 2D models have significant limitations in considering mechanical effects (i.e. shear caused contacts/closure) and nonlinear flow behavior (i.e. transverse and eddy flows). These limitations have not been systematically presented and discussed.

The impacts of shear caused aperture changes and contact spots, as well as strong inertial effects on nonlinear flows in 3D rough-walled fractures motivated this study. We presented the numerical modeling results of fluid flow through realistic rough-walled fracture models in 3D, by directly solving the NSE, to investigate the impacts of shear and detailed nonlinear fluid flow behaviors, so that the limitations of 2D simplifications can be clearly demonstrated, and the validity of the LCL approaches for transmissivity evaluations in 3D rough-walled fractures can be quantitatively analyzed. The results can advance our understanding in nonlinear fluid flow in natural fractured rocks, which is relevant to many rock engineering practices and underground projects.

The originality of this study lies in three aspects: 1) nonlinear flow fields in the 3D rough-walled fractures enhanced by shear caused variable aperture space and contact spots; 2) statistical analysis of relations between effective transmissivity and apertures, which may provide new insights into the uncertainties of evaluating permeability of fractured rock masses, and 3) detailed analysis of limitations of 2D models in modeling of nonlinear flow behaviors in rough-walled fractures.

2 Fracture geometry model with mechanical effects

2.1 Geometry model of 3D rock fractures

A laser-scanned natural granite rock fracture surface was used as the parent surface for creating 3D fracture models for roughness representation and fluid flow modeling. The size of original rock specimen is 0.1 m in width and 0.2 m in length. The topographical data of the sample surface were obtained with an interval of 0.2 mm in both x- and y-axis with an accuracy of $\pm 20 \mu\text{m}$ and a resolution of $10 \mu\text{m}$ (Fig. 1a) [21].

Limited by the challenging computational capacity of solving the NSE for the 3D fracture models with highly fine representation of surface roughness, only a part of the surface at the zone of $x = [40, 64.8] \text{ mm}$ and $y = [25, 49.8] \text{ mm}$ (with the size of 24.8 mm in length and 24.8 mm in width) were cut out to form the 3D models for a generic study (Fig.1a-d). This part was chosen in order to avoid the effects of sample edges as well as the extreme asperity heights, thus to avoid only single asperity contact spot appearing in the computational model. The topographical interval of the surface is $I_x = I_y = 0.4 \text{ mm}$, which is an upscaling

Fig. 1 Scanned rock surface and geometry of the 3D fracture models: (a) the laser-scanned natural granite rock surface; (b) lower surface; (c) geometry of the model M1; (d) geometry of the model M2; (e) top view of the model M2. Contact spots highlighted as white spots in d), but red spots in e) of model M2.

from the original laser scanned data (with topographical interval of 0.2 mm) but provided a proper representation of surface roughness. This upscaling practice has been commonly adopted in 3D modeling to reduce the difficulty of meshing and computational loads [12, 35].

Two 3D fracture models, one with and another without the shear caused asperity contacts, were created for simulations, so that the shear effects can be clearly demonstrated by comparison between results from the two models. The first model, M1, was built by a numerical ‘lift’ step that simply extruded the scanned surface upwards in the vertical (height) direction (z-direction) by 0.65 mm (Fig. 1a-c). Therefore, the vertical aperture of the model M1 is a constant of 0.65 mm, without asperity contacts at all. The second model, M2, was

Fig. 2 Cross-sections on z - y plane at $x = 12.5$ mm, showing significant difference in aperture spaces between model M1 and M2: (a) model M1 (b) model M2.

created numerically by a ‘shear’ step along the horizontal length direction (x -direction) with a displacement of 1.0 mm, after the same ‘lift’ step used for creating model M1 (Fig. 1d-e). This ‘numerical shear’ step created a numerical 3D fracture model with changing apertures formed by the unmatched upper and lower surfaces, which performs like a simplified shear test commonly conducted in laboratory tests of rock fractures, under small or no normal compression but with shear dilations at asperity contact spots. Note that this ‘numerical shear’ was not received from physically realistic laboratory tests, but provided realistic fracture model geometry with contacting asperities and complex space of varying apertures everywhere in the model M2.

In order to clearly show the significant difference between M1 and M2 models, two cross-sections on z - y plane at $x = 12.5$ mm (see Fig. 1c and d), taken from the two models, respectively, were presented in Fig. 2. The model M1 is similar to the 2D fracture models commonly found in literature without contact spots between upper and lower surfaces, but with a uniform vertical aperture (Fig. 2a). Fig. 2b shows location and geometry of the vertical cross-sections of two asperity contacts. Since the two models were created based on the same wall surface topography, the impacts of shear can be clearly compared on a more logically valid basis.

The 3D fracture models constructed in the way as presented above were artificial, since laboratory tests of fractures (in size of ~ 25 mm) with measurements of compression, shear and nonlinear fluid flow monitoring at micro-millimeter scales are not available. The modelling results, however, can serve for realistic conceptual understanding of the physical

behavior of nonlinear flow in natural rough-walled rock fractures with shear and its resulting impacts on mass transport processes.

2.2 Fracture characterization

The flow behaviors in fractures depend on the geometry characteristics, commonly characterized by the mid-surface and aperture geometry. The mid-surface is often used to roughly characterize the tortuous flow paths in the vertical direction (z-axis). The aperture space determines the fluid flow passes, which directly determines the transmissivity and flow-wetted areas.

For model M1, the vertical apparent aperture is a constant of 0.65 mm and the mid-surface is of the same shape as its lower and upper surfaces. For model M2, the mid-surface is the mean height of the lower and upper surfaces. The 1.0 mm shear displacement changed aperture from constant to varying over the whole fracture model. Fig. 3 shows the spatial and density distribution of apertures of the model M2. The local apertures are discretely distributed along the aperture space, but show good connectivity (Fig. 3a). Small aperture zones (blue areas) are shown around the contacting spots of zero apertures (small white squares in Fig. 3a). Such discrete distribution of apertures resulted in a heterogeneous distribution of transmissivity, which is the reason for the complicate preferential or channeling flow behaviors in the rough fractures, as shown and discussed in Section 4.

The Chi-Square goodness-of-fit method is commonly used to determine the best probability density function (PDF) to fit the density distributions. The goodness-of-fit is defined as a chi-square random variable (χ^2), expressed as:

$$\chi^2 = \sum_{i=1}^N (O_i - E_i)^2 / E_i \quad (1)$$

where N is the number of bins, i is an integer from 1 to N , O_i are the observed counts and E_i

Fig. 3 Aperture distributions of model M2: (a) space distribution of apertures; (b) histogram of the aperture.

are the expected counts based on the hypothesized distribution. The lower value of χ^2 refers to the better fitting of observed data through the hypothesized distribution. After a trial-and-error test using the MATLAB statistics toolbox [36], the Normal PDF was the best fitting function for the apertures density distribution, with mean value of $\mu = 0.65$ mm and standard deviation $\sigma = 0.22$ mm (Fig. 3b). Note that the mean value is equal to the up-lift distance of 0.65 mm, same as the constant aperture of model M1, due to the small shear displacement applied. This, however, serves as a good basis for comparison of the results between the two models.

3 Modeling of fluid flow

3.1 Governing equations and numerical methods

The governing equations of flow are the NSE which represents mass and momentum conservations. For the isothermal, steady-state and incompressible single Newtonian fluid flow, The NSE can be written as

$$\nabla \cdot \mathbf{u} = 0 \quad (2)$$

$$\rho(\mathbf{u} \cdot \nabla)\mathbf{u} - \mu \nabla^2 \mathbf{u} = -\nabla P \quad (3)$$

where ρ (kg/m³), $\mathbf{u}$ (m/s), P (Pa), μ (Pa · s) and t (s) denote the density of a fluid, the velocity vector, the pressure, the viscosity coefficient and time, respectively.

The NSE is a set of nonlinear partial differential equations coupled with velocity and pressure fields. In this study, the commercial finite element software of COMSOL Multiphysics was employed to solve the NSE [37].

3.2 Initial and boundary conditions

For numerical simulations, meshes of around 1.2 million tetrahedral elements were used for discretization of the model M1 and M2. The number of elements was selected through a sensitivity analysis process in order to obtain mesh-independency of the results.

For comparisons, the initial and boundary conditions of the two models were set as the same. The two boundaries at $y=0$ mm and $y=24.8$ mm were set as the inlet and outlet boundaries, respectively (Fig. 1c and d). The inlet boundary conditions were specified with different values of constant flowrates, Q (m³/s), and the outlet boundary condition was set as zero pressure, i.e. $P = 0$ Pa. The rest of top, bottom, side boundaries in the two models were set as no fluid flow and non-slip walls, i.e. $\mathbf{u} = 0$ m/s. Such boundary conditions are consistent with many laboratory experiment conditions [19]. To reduce the inlet boundary effects of constant flowrate (which often lead to constant velocity), a laminar entrance inflow condition, provided by the COMSOL software, was adopt in all simulations [37]. Using this laminar entrance inflow condition can largely improve the convergence rates, especially in nonlinear

flow cases when Re is relatively high. With such settings, the y -axis direction is the principal direction of fluid flow.

In order to investigate the effects of flow conditions on the transmissivity evaluation, five laminar entrance inflow conditions with different flowrates ($Q1 = 1.3074 \times 10^{-8} \text{ m}^3/\text{s}$, $Q2 = 1.3074 \times 10^{-7} \text{ m}^3/\text{s}$, $Q3 = 1.3074 \times 10^{-6} \text{ m}^3/\text{s}$, $Q4 = 6.5370 \times 10^{-6} \text{ m}^3/\text{s}$ and $Q5 = 1.3074 \times 10^{-5} \text{ m}^3/\text{s}$) were adopted in this study, leading to five Re values at the inlet boundaries. A commonly used definition of Re in rock mechanics and geophysics communities was adopted as [20]

$$Re = \frac{\rho \bar{u} \hat{b}}{W \mu} = \frac{\rho Q}{W \mu} \quad (4)$$

where $\bar{u}(\text{m/s})$ is the mean velocity, $\hat{b}(\text{m})$ is the characteristic length approximated by the mean fracture aperture, $W(\text{m})$ is the width of fracture and $Q(\text{m}^3/\text{s})$ is the volumetric flowrate. The density and viscosity of water were taken as $\rho = 0.9997 \times 10^3 \text{ kg/m}^3$ and $\mu = 1.307 \times 10^{-3} \text{ Pa} \cdot \text{s}$ (water at 10°C), respectively. With the settings of five flowrate at inlet boundaries, the corresponding Re numbers are 0.4, 4.0, 40.0, 200.0 and 400.0, respectively. Such ranges of Re numbers exist in groundwater flows in rock engineering in mountain areas, hydraulic engineering, pumping/slug tests and laboratory experiments [12-13, 15-17]. More comprehensive discussion on the range of Re is provided in Section 6.

4 Results of flow complexity in 3D rough-walled fractures

4.1 Flow velocity

The simulated flow velocity fields in the y -direction, u_y , for the two fracture models, with $Re = 0.4, 40.0$ and 400.0 , are shown in Fig. 4.

Comparing the results of the two fracture models, u_y in model M2 was distributed more non-uniformly and channelized than that of the model M1, and the magnitude range of u_y in model M2 is almost twice as that in the model M1, caused by increased complicity of flow field due to aperture changes and asperity contacts by shear. In model M1 (Fig. 4a, c and e), low velocity zones (blue colored areas) were located around a few large asperities of sharp corners, (see Fig. 2a). These large asperities mainly increased the tortuosity of flow in the vertical direction (z -axis), as shown in Fig. 4c and caused small zones of reverse/eddy flows with negative u_y values at such large asperity locations, with higher Re values (Fig. 4e). In model M2 (Fig. 4b, d and f), low velocity zones generally located around the contact spots of zero transmissibility (see also Fig. 3a), where the fluids were forced to flow around them, with clear tortuous flow features. Such forced tortuous flow features resulted in dispersal flow paths in all three coordinate directions (x -, y - and z -axis), which therefore significantly

Fig. 4 Principal velocity in y-direction for the 3D fracture models with different Re . (a) $Re = 0.4$, model M1; (b) $Re = 0.4$, model M2; (c) $Re = 40.0$, model M1; (d) $Re = 40.0$, model M2; (e) $Re = 400.0$, model M1 and (f) $Re = 400.0$, model M2.

increased the flow tortuosity in whole aperture space, with increasing variations of Re values. The negative u_y value in Fig. 4f, with $Re = 400.0$, also indicates existence of nonlinear reverse/eddy flows in the fracture model M2.

4.2 Streamlines showing channeling transverse and eddy flows

The streamlines of flow fields in the two extreme cases, $Re = 0.4$ and 400.0 , were exemplified in Fig. 5, to show overall trends of pathways of fluid flow through the 3D rough-walled fracture model, with contour maps presenting the norms of the velocity magnitude

field ($|U| = \sqrt{u_x^2 + u_y^2 + u_z^2}$, where u_x , u_y and u_z is the x, y and z components of velocity).

The sliced contour maps also serve as the geometry background for the streamline distributions in space.

Comparing the two fracture models, the streamline distributions of model M1 were generally homogenous with paralleled lines along the principal flow direction (shown by the

Fig. 5 Streamlines of flow in the 3D fracture models with different flowrates/ Re . (a) $Re=0.4$, model M1; (c) $Re = 400.0$, model M1; (e) $Re = 0.4$, model M2 and (g) $Re = 400.0$, model M2. (b), (d), (f) and (h) is the top view of (a), (c), (e) and (g), respectively.

arrow in black color), but that of model M2 were much channelized with significant tortuosity, dominated by the locations of the contact spots created by shear, despite the fact that the topography of the wall surfaces of the two models are identical.

Note that even in model M1, a small scale eddy flow at a sharp corner on the upper surface with large asperities (see location on Fig. 2a and Fig. 5c) when $Re = 400.0$, see Fig. 6a and b. This kind of eddy flow is not the closed-streamline eddy flows observed in 2D models [23, 25], but a local whirling backflow with open streamlines towards the main flow direction. This finding indicated an important limitation of 2D modeling for such nonlinear flows in rock fractures, which is further discussed in Section 6.

In contrast, the streamlines of model M2 (Fig. 5e-h) clearly demonstrated the complicate channeling flow along the preferential paths, around the contact spots and the widely distributed eddy flows when $Re = 400.0$ (Fig. 5h). The streamlines are much tortuous and concentrated in a few fast flowing channels with higher velocities around the contact spots (Fig. 5e-h). Comparing the streamlines in different Re values for model M2 (Fig. 5f and h), the streamlines are less tortuous but more concentrated to form less number of channels of higher velocity, with higher Re number ($Re = 400.0$), demonstrating strong inertial effects.

The most significant differences of eddy flow features between the two models when $Re = 400.0$ are the locations and geometrical features. Two examples of zoomed-in streamlines of eddy flows were presented in Fig. 6. In model M1, the eddy flow streamlines occurs at the low velocity zone of the sharp corner of the upper surface (Fig. 6a and b), showing continuous open streamlines in 3D into and out the sharp corner with a strong whirling motion in the vertical direction (Fig. 6a). Its formation mechanism shows a similarity with typically eddy flow in sharp corner of rough surfaces observed in other numerical studies (Fig. 6b) [23, 25] and experimental investigations [17-18]. At the same location but with two surfaces contacted near the large asperity, in model M2, the eddy flows mostly located in horizontal directions behind the contact spot, occupying much larger space sizes and more complicate streamline shapes (Fig. 6c and d). Its formation mechanism is similar to the classical viscous flow passing around a cylinder column in fluid dynamics [38], but with more complicated geometry shapes due to the non-uniform geometry of the contact spot formed by the large asperity during the shear process. It is also worth to mentioning that the characters and patterns of such complicate eddy flows in both model M1 and M2 cannot be well represented by any 2D models, which is very different compared with 2D model results of the same basis of fracture surface geometry as shown in Ref. [25]. More comprehensive discussion is given in Section 6.

Fig. 6 Enlarged zoomed-in views of complex features of flow streamlines in 3D, around a large asperity of sharp corner on the surfaces of the fracture, of the two models when $Re = 400.0$: (a) Streamlines of model M1 without contact spot, vertical view in direction perpendicular to the horizontal X-Y plane (birds view); (b) horizontal front view of model M1 along the direction perpendicular to the vertical Y-Z plane; (c) Streamlines of model M2 around a large asperity contact spot in the vertical direction perpendicular to the horizontal X-Y plane (birds view) and (d) horizontal front view of model M2 along the direction perpendicular to vertical Y-Z plane.

To sum up, such significant difference between the results of two fracture models indicated the important effects of geometry structure changes, mainly aperture space variation and contact spots caused by shear. The large difference in flow field with different Re numbers in model M2 (Fig. 5e-f and Fig. 5g-h) demonstrated the combined effects of mechanical loading on the changes of fracture geometry and inertial/nonlinear term on the nonlinear flow behaviors in 3D rough-walled fractures.

4.3 Pressure and nonlinear relation with flowrates

Pressure field is another important variable in solving of the NSE, which is also required for estimating effective transmissivity through the LCL approach. The pressure fields of the two models are presented in Fig. 7, exemplified when $Re = 400$.

In both models, the pressure values decrease along the y-axis direction, and distribute non-uniformly along the x-axis direction, especially in model M2 (Fig. 7b), due to the surface roughness, contact spots and change of aperture space. The pressure on the inlet boundary is not constant but with a small range of variation because of the flowrate inlet boundary condition, as shown in Fig. 7 and described below.

In the CL or LCL models, the flowrate, Q (m^3/s), is linearly related to the pressure gradient. However, for nonlinear flows, the impacts of surface roughness and inertial term result in nonlinear relationship between the flowrate (Q) and the pressure gradient (∇P), which can be described by nonlinear formula (i.e. Forchheimer's law) expressed as:

$$\nabla P = \frac{\overline{P_{inlet}} - \overline{P_{outlet}}}{L} = AQ + BQ^2 \quad (5)$$

where A and B are the fitting coefficients represent energy losses due to viscous and inertial dissipation mechanisms, respectively, according to the Forchheimer's law[16]. The pressure gradient was calculated from the averaged pressure on the inlet ($\overline{P_{inlet}}$) and outlet ($\overline{P_{outlet}}$) boundaries. The pressure on the outlet boundary was set as zero ($\overline{P_{outlet}} = 0$). The variations of pressure along the inlet boundary are very small even when $Re = 400$, with the coefficient of variation (ratio of the standard deviation over the mean value) equals to 0.0160 for M1 and 0.0113 for M2, respectively (see Fig. 7). Therefore, using averaged pressure along the inlet boundary is acceptable.

Based on the mean pressure values along the inlet boundary and zero pressure along

Fig. 7 Pressure fields when $Re = 400$, for (a) model M1 and (b) model M2. The coefficient of variation (ratio of the standard deviation to the mean) of the pressure on the inlet boundary equals to 0.0160 and 0.0113 for the model M1 and M2, respectively.

Fig. 8 Nonlinear relationships between flowrates and pressure gradients.

the outlet boundary of the two fracture models, the pressure gradients varying versus the flowrates were plotted in Fig. 8, showing strong nonlinearity between the flowrates and pressure gradients in both models M1 and M2, that can be mathematically represented by Eq. 5 with different A and B parameters. The differences between two curves indicated that variable apertures and contact spots significantly increased the nonlinearity of flow in 3D rough-walled fractures. The curves represented by Eq. 5 fit well with the Forchheimer's law. However, the quantitative correlation function between its coefficients and the fracture geometry conditions require further studies in the future [19].

5 Effective transmissivity with local apertures

5.1 Effective transmissivity with LCL

When the LCL is adopted, each interval of surface roughness (I_X or I_Y) can be recognized as a local flow cell, and the local transmissivity on the roughness scale can be expressed as a function of the local aperture. In the y -direction (principal flow direction for this analysis), the local transmissivity, T_{y_i} (m^2/s) can be expressed by the averaged aperture $\bar{b}_f(y_i)$ of the flow cell y_i , written as

$$T_{y_i} = \frac{\bar{b}_f(y_i)^3 \rho g}{12\mu} \quad (6)$$

The best approximation of averaged aperture on local scale was estimated from harmonic mean of adjacent apertures of the flow cell $b_f(y_i)$ and $b_f(y_{i+1})$, written as [11],

$$\bar{b}_f(y_i)^3 = \frac{2 b_f(y_{i+1})^3 b_f(y_i)^3}{b_f(y_{i+1})^3 + b_f(y_i)^3} \quad (7)$$

In Ge [6], the aperture calculation considered vertical tortuous flow along the mid-surface, which led to a modified aperture by projection on the mid-surface, given by

$$b_f(y_i) = b(y_i) \cos \phi_{y_i} \quad (8)$$

where the $b(y_i)$ is the vertical aperture and ϕ_{y_i} is the local slope angle of the mid-surface along the y-axis direction.

Based on above concepts, the LCL approach of effective transmissivity can be inversely evaluated from flow and pressure results that were obtained by solving NSE. In this study, the velocity in the middle of flow cells and pressure on the two sides of flow cells along the modified aperture (Eq. 8) were linearly interpolated from flow and pressure fields by using the built-in spatial interpolation algorithm of MATLAB [36]. Then, the interpolated velocity and pressure were used to calculate the averaged velocity $\overline{u_{y_i}}$ and pressure gradient ∇P_y across the modified aperture. The local effective transmissivity $T_{y_i}^e$ projected on the local mid-surface then was obtained in form of

$$T_{y_i}^e = \frac{\rho g \bar{b}_f(y_i) \overline{u_{y_i}}}{\nabla P_y \cos \phi_{y_i}} \quad (9)$$

Based on Eq. 9, the effective transmissivity of the two fracture models with different Re numbers were calculated for statistical analysis, as described below.

5.2 Statistics of effective transmissivity

Statistical indices of mean, standard derivation, skewness and kurtosis of the effective transmissivity are presented in Table 1.

Table 1 Statistical indices of effective transmissivity, T (m^2/s).

Re	Mean (M1 / M2)	Standard deviation (M1 / M2)	Skewness (M1 / M2)	Kurtosis (M1 / M2)
0.4	1.31e-4 / 1.67e-4	1.98e-5 / 1.37e-4	1.61 / 1.42	6.50 / 5.57
4.0	1.31e-4 / 1.67e-4	1.96e-5 / 1.41e-4	1.58 / 1.58	6.45 / 5.68
40.0	1.07e-4 / 3.13e-4	2.38e-5 / 2.53e-3	3.81 / 28.27	7.20 / 60.64
200.0	5.01e-5 / 3.48e-5	6.20e-5 / 1.05e-3	25.55 / 21.40	84.75 / 88.47
400.0	3.12e-5 / 1.43e-5	5.13e-5 / 1.38e-2	28.69 / 50.64	108.58 / 257.26

The mean values of effective transmissivity in both fracture models significantly decrease with the increase of Re from 0.4 to 400.0, especially when $Re \geq 40.0$. In the whole range of Re, the standard derivations of effective transmissivity of model M2 are generally larger than that of model M1, indicating the more heterogeneous character of the model M2,

because of the complex geometry conditions caused by the shear process. Both skewness and kurtosis values increase significantly with increasing Re , indicating decreasing effective transmissivity with increasing Re , due to the increasing inertial effects.

Fig. 9 Scatter plots of effective transmissivity with apertures. (a) $Re = 0.4$; (b) $Re = 4.0$; (c) $Re = 40.0$; (d) $Re = 200.0$ and (e) $Re = 400.0$.

Note that although the aperture is constant in model M1 and nearly following the normal distribution in model M2 (see Fig. 2b), the effective transmissivity of both model shown strong skewness and kurtosis, which is consistent with field observations that the transmissivity often obey log-normal or Pareto distributions [39]. Such strong skewness and kurtosis also indicate the heterogeneous feature of transmissivity in 3D rough-walled fractures.

Fig. 9 presents the scatter plots of the effective transmissivity with respect to the local aperture of the 3D fracture models with different Re . The theoretical relation between transmissivity and apertures based on the LCL was also plotted in Fig. 9 for comparison. Note that due to the constant vertical aperture (0.65 mm) of model M1, transmissivity values of model M1 stops at aperture value of 0.65 mm (shown in green dots in Fig. 9).

As shown in Fig. 9, scatter plots of local effective transmissivity versus local apertures for both fracture models M1 and M2 are strongly correlated when $Re \leq 4.0$ (Fig. 9a and b). The scatter points were generally following the trends of LCL model results (blue curves), with a possible representative effective transmissivity curves in a statistical sense. However, the scatter points were more widely distributed with increasing derivations when aperture values increase, indicated that effective transmissivity of the 3D rough-walled fractures, calculated using LCL approach, cannot be represented approximately by a deterministic function of aperture. The results of LCL (blue lines) in Fig. 9a-b are generally close to upper bonds of effective transmissivity point clouds, indicated the LCL approach generally overestimated the transmissivity of fractures, even when Re is small (i.e. $Re = 0.4$). The main reason is that the corrected LCL model (using Eqs. 6-8) still cannot fully capture impacts of channeling and transverse flows in the x-direction, since these two issues were not considered in the LCL approach. Particularly, effective transmissivity of the fast flow channels is larger than the LCL estimations, but effective transmissivity of most transverse flow zones is smaller than the LCL estimations due to increased tortuosity of transverse flows. In Fig. 9c-e, the mean effective transmissivity points significantly wide-spread with larger range of derivations and increased transmissivity values with increasing Re , indicating the failure of LCL approach with highly nonlinear flow fields, due to its basic assumption of laminar or approximately laminar flow conditions.

Comparing results of the two fracture models, the distribution of effective transmissivity of model M1 is slightly better in agreement of LCL than that in model M2 when $Re \leq 4.0$, indicating that even for open fractures of complex roughness of surfaces, the effective transmissivity based on LCL approach is valid only when Re number is adequately

small, and mechanical effects by shear increases limitations of LCL for rough-walled fractures.

To quantify the differences between the effective transmissivity and LCL approach estimations, their relative differences (RD) were calculated and presented in a Box-and-whisker plot (Fig. 10). The RD is expressed as:

$$RD = \frac{T_{y_i}^e - T_{y_i}^{LCL}}{T_{y_i}^{LCL}} \times 100\% \quad (10)$$

The Box-and-Whisker plots in Fig.10 quantitatively present the medians (red line in boxes), quartiles (blue boxes), ranges (dashed line out of box) and extreme values (green or red dots) of the RD between the effective transmissivity and LCL approximation.

For model M1, when $Re = 0.4$ and 4.0 , the median RD comparing with the LCL are around -15% . The magnitude of RD increases to around 80% with the increasing Re numbers from 40.0 to 400.0 .

For model M2, when $Re = 0.4$ and 4.0 , the median RD are around -15% . Similar with model M1, the magnitudes of RD of model M2 also significantly increases to 90% with the increasing Re numbers, but with wider ranges and more extreme values than that of model M1.

Such results indicate that the LCL is a poor approach for modeling fluid flow in 3D rough-walled fractures, even with small Re numbers, as in such a simple fracture model as M1. Therefore, care should be taken when using LCL approach for fluid flow in fractures or fracture networks, and with respect to the initial and boundary conditions of the problems, which may cause possible changes of Re values.

In summary, the statistics of effective transmissivity calculated from numerical

Fig. 10 Relative differences (RD) illustrated by Box-and-Whisker plots: (a) model M1 and (b) model M2.

modeling of nonlinear flow in the 3D rough-walled fractures can provide detailed information for the uncertainty analysis of the relations between effective transmissivity and apertures, and indicated the limitations or advantages of the models, such as LCL and NSE models. The main reason of such uncertain relationship between the transmissivity and aperture is that in realistic natural fractures, effective transmissivity is not only determined by local apertures at specific locations, but also affected by neighboring aperture geometry structures, as well as nearby flow conditions. It is affected by the combination of both effects of the complex geometry conditions (i.e. variable apertures, surface roughness and contact spots) and flow behaviors (i.e. channeling, transverse and eddy flows) or even more complicated physical and chemical processes at both local and close neighborhoods.

Quantification of representative transmissivity is an important issue in rock physics and engineering practices. The finding presented above provided new insights into the uncertainty issue of the transmissivity in 3D rough-walled fractures from a statistical perspective, showing uncertainties of effective transmissivity and limitations of LCL assumptions that are commonly applied for problems of fluid flow through natural fractured rocks in practices.

6 Discussions

6.1 Comparison with previous studies

In this study, we presented the numerical simulations of nonlinear flow in two 3D rough-walled fracture models by directly solving the NSE, with focuses on the mechanical impacts (shear) on aperture changes and asperity contacts. We also analyzed the relations between effective transmissivity and local apertures in the 3D fracture models of realistic surface roughness features with varying fluid flow behaviors, from nearly laminar to nonlinear with increasing inertial effects (Re numbers). The complex nonlinear flow fields (represented by streamlines) at the neighborhoods of asperity contacts and quantitative demonstration of limitations of LCL approach for estimating effective transmissivity presented in this study are two important issues that have not been adequately investigated so far.

Fracture surface roughness and mechanical effects on aperture space changes are important issues, which significantly increased the complexity of flow behavior in natural 3D fractures. This was shown by the results and interpretations presented above. However, it is a difficult challenge for laboratory experiments to illustrate this without adequate visualization techniques. Detailed illustrations of complex flow features around contact spots, in 3D, are presented in this paper, and have rarely appeared in previous related literature [12- 14, 34-35].

Comparing with a recent 3D study in Ref. [8], we focused on the nonlinear flow behavior, considered inertial effects and significant impacts of asperity contacts caused by shear process. In such cases with complex geometry and flow conditions, it was difficult to find the meaningful and general correction factor as reported in Ref. [8]. The reasons are that, on one hand, the realistic geometry structures of 3D fractures cannot be simplified or generalized into simple 2D or 3D models of regularly-shaped wedges. On the other hand, the shear enhanced nonlinear flows, such as channeling, transverse and eddy flows with strong inertial effects, were significantly beyond the capability of the LCL approach. Therefore, such correction factor in modified LCL approach for nonlinear flow is only empirical and may bring more unknown uncertainties.

6.2 Re numbers of fracture flow and connection with applications

In natural and engineering projects, the state of fluid flow through fractured rocks may vary from laminar to turbulent flows, depending on both hydraulic gradients and fracture geometry structures. The ranges of Re between 0.4 and 400.0 in this study covers both laminar flows (i.e. $Re \leq 4.0$) and complicated eddy flows (i.e. $Re = 400.0$), which commonly exists in many engineering projects, such as hydraulic engineering, mining and geothermal extraction [40], as well as laboratory experiments [12, 14-16, 19, 35].

Particularly, our results are closely relevant to pumping and slug tests which are the primary *in situ* tests in field to obtain the transmissivity information of the subsurface. For instance, in pumping test, the effective transmissivity values were also inversely estimated from the measured pumping flowrates and dropdown of hydraulic head. For the fractured-rock aquifers, the dropdown response in observation wells is mostly dependent upon the fracture distributions (i.e., density, orientation, length, aperture and roughness, and connectivity), rather than the radial distance in mostly homogenous porous media [41]. With specific operation flowrates and aquifers conditions, the nonlinear flows often occur in pumping and slug tests, especially in fractured-rock aquifers [42-43]. The effective transmissivity results presented in this study showed the flowrate/ Re dependent characteristics of effective transmissivity in rock fractures, where the effective transmissivity values generally decrease with increasing flowrate/ Re , due to the nonlinear flow behaviors. Such flowrate/ Re dependent characteristics of effective transmissivity may also exist in pumping test at fractured-rock aquifers when nonlinear or even turbulent flow occurs. Therefore, to obtain realistic effective transmissivity values, it is important to choose the proper pumping rate according the operational flowrate in applications.

The critical Re or hydraulic gradients for the fracture flow transition from linear regimes into nonlinear regimes have been intensively reported and discussed in literature [12-13, 15-17, 40]. However, the reported critical Re values are varying in large ranges from around 1 to 2300 in different publications, indicating that no standard constant critical Re numbers for fracture flow exist, due to the different fracture geometry structures (i.e. aperture spaces and surface roughness) and boundary conditions. In addition, the commonly used definition of Re (see Eq. 4) is deficient in the characteristic length that is often given as the mean aperture. However, the mean aperture is estimated on the total scale of fractures, which is a poor representation of the characteristic length for rough-walled fractures. It is known that the eddy flows often occur at local scales where sharp asperities of the surfaces and contact spots were contained as shown in this study and in experimental observations [17-18]. Therefore, any critical Re numbers for nonlinear flow in fractures should be subjective to the specific fracture geometry structures (especially the local aperture spaces and surface roughness) and conditions of the problem concerned in applications.

6.3 Limitations of 2D models and impacts on mass/heat transport

Due to the difficulties in solving NSE for modeling flow in 3D rough rock fractures with complicate geometry conditions, traditional studies often simplified the 3D rock fractures into 2D problems by ignoring the vertical flow in z-axis direction [30], or ignoring the transverse flow in x- or y-axis direction [21, 23-25]. Although such simplified 2D fracture models provided some important conceptual understandings of surface roughness effects on flow complexity and impacts on transport processes in fractured rocks, the 2D models have significant limitations.

In the simplified 2D fracture models by ignoring vertical flows (in z-axis direction), the significant impacts of mid-surface roughness or the vertical tortuosity could not be considered. Similarly, in the simplified 2D fracture models representing a vertical cross-section of fracture by ignoring flow in one horizontal direction (transverse flows in x- or y-axis direction), it is not possible to consider the impacts of mechanical loading caused contact spots between two surfaces of the fracture model. It is also not able to model the nonlinear channeling and transverse flow behaviors. Another typical example in this type of simplified 2D fracture models is that the fluid was forced to flow faster at the zones with smaller apertures due to the mass conservation requirement. However, 3D simulations showed that the lower velocity zones may also largely located around the contact spots with smaller apertures, as shown in Fig. 4b, d and f, required by mass conservation law.

Particularly, the simplified 2D fracture models have fundamental limitations in modeling of eddy flows. Ideal eddy flows represented by closed-streamline in areas of large geometry changes, such as sharp corners of surfaces, are observed often in 2D fracture models formed by a cross-section of two opposite surfaces, as published in many publications (see the Ref. [30], as a recent example). However, in 3D models (e.g. model M1 and M2 in this paper) established on the same parent fracture surface, the eddy flows were shown as complicated whirling reverse flow with open streamlines (see Fig. 6). This observation indicates that the ideal eddy flows of closed-streamline in 2D rock fracture models are most likely caused by the 2D assumptions, but may not exist in real 3D rough-walled rock fractures due to complex geometry conditions, especially variable aperture space in another horizontal direction.

In order to clearly demonstrate correctness of the above understanding for eddy flows in fractures, two 3D fracture examples, one with a single tetrahedral asperity, another

Fig. 11 Examples with single asperity illustrating the limitations of 2D models in modeling of nonlinear flows in fractures: (a) simplified model with a single tetrahedral asperity; (b) simplified model with a long triangular prism asperity; (c) complicate eddy flows in the tetrahedral asperity and (d) closed-streamline eddy flows shown in 2D fracture models at the central section of the 3D model on the y-z plane at the central symmetric cross-section.

one with a triangular prism asperity, were calculated and presented in Fig. 11. The first example represents an idealized tetrahedral asperity space on the upper surface of the fracture model (Fig. 11a). The second example illustrates an idealized long asperity space of constant triangle cross-section but extruded along the x-direction in a shape of triangular prism on the upper surface of the fracture model (Fig. 11b). With the similar initial and boundary condition settings described in Section 3.2, the flow features expressed by streamlines in the neighborhoods of the asperities in both example models are shown in Fig. 11c and d, respectively.

Obviously, the flow features in the first model shows complicated whirling backflows and transverse flows, which cannot be simplified into any 2D planes. In contrast, the streamlines in the second model shows more regular closed-streamline rotational flows on the central cross-section of y-z plane of the model, typically appear in 2D fracture models for solving NSE. Only in this case, the eddy feature could be described by the simplified 2D plane of symmetric geometry model since the assumption of the prism has infinite lengths in theory for 2D problems. In reality, however, such constant asperity geometry along the extrusion direction does not exist in natural rock fracture surfaces in general.

In literature, such closed-streamline Eddies shown in Fig. 11d are often treated as ‘stagnant water zones’ where fluid advections were ignored since the water was considered to be fully trapped. In reality, such as shown Fig. 11c, open 3D Eddies formed advection paths, so that water was not fully trapped but also flow out from the eddy zones. This issue will become more important for solute transport modelling, when advection is the dominant transport mechanism, such as in the field of radioactive waste disposal in fractured crystalline rocks, since where the connected fracture network dominates water flow and advection is one of the major transport mechanisms affecting the final breakthrough results. A recent study reported in Ref. [18] also found that the eddy in rough-walled fractures have significant impacts on the tails of solute transport breakthrough curves through both experimental observations and numerical modeling of a simplified geometry model with single asperity similar to the examples shown in Fig. 11a. It is also worth to note that the complicated eddy flows would also affect the local interactions between fluid/solute and the rock matrix, e.g. sorption, matrix diffusion and chemical reaction processes.

The results obtained from the above demonstrative examples showed that the limitations of 2D model for fluid flow in rough-walled fractures is an important issue that has to be considered, because the ideal stagnant eddy flow presented by closed-streamline circles

occurs in 2D models most possibly may not occur in reality, besides that the 2D models are unable to properly consider effects of mechanical loading processes.

7 Concluding remarks

Some general conclusions of importance extracted from this study are summarized below:

In rough-walled fractures, even with the same conditions of surfaces roughness and mean aperture values, the mechanical processes, especially the shear processes, caused aperture space variations and contact spots, which significantly affect the nonlinearity of flow behaviors, resulting in complicated channeling, transverse and eddy flows.

Besides of the geometry conditions affected by mechanical loadings, the inertial effects represented by Re is another important factor for the nonlinear flows, e.g. the complicated eddy flows when $Re = 400.0$ in this study. It showed strong inertial effects in 3D rough-walled fractures. In addition, Re is not an independent and unique constant that determines the nonlinear flow behavior, but always combined with specific geometry structures and boundary conditions. Therefore, it would be more useful and reliable to define critical Re numbers for nonlinear flow base on specific problems/conditions in applications.

The relationship between total flowrates and pressure gradients were shown with strong nonlinearity, which can be well described by the Forchheimer's law. The effective transmissivity was found strongly related to local apertures, when Re is small ($Re < 4.0$ in this study), since then the relationship between effective transmissivity and local apertures could approximately follow the trend of LCL model predictions. However, their relationship closely depends on inertial effects (Re) and impacts of other conditions such as combined effects of mechanical processes, geometry conditions (i.e. surface roughness, variable apertures and contacting spots).

The modeling results illustrated limitations of 2D fracture models and importance of applying 3D models of fluid flow in rough-walled rock fractures, then significant impacts of geometry conditions, such as surfaces roughness evolutions and mechanical loading processes can be correctly considered and understood. However, it requires considerable increase of computational capacity and effectiveness.

The major challenge is the adequate laboratory experiments for flow and mass transport under mechanical loading with adequate resolution and accuracy of data measurements and visualization, which does not exist at present. Therefore, numerical results presented in this study cannot be validated properly, but can be used to help such experimental designs in the future.

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