Numerical modeling of the effects of roughness on flow and eddy formation in fractures

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The effect of roughness on flow in fractures was investigated using lattice Boltzmann method (LBM). Simulations were conducted for both statistically generated hypothetical fractures and a natural dolomite fracture. The effect of increasing roughness on effective hydraulic aperture, Izbash and Forchheimer parameters with increasing Reynolds number ($Re$) ranging from 0.01 to 500 was examined. The growth of complex flow features, such as eddies arising near the fracture surface, was directly associated with changes in surface roughness. Rapid eddy growth above $Re$ values of 1, followed by less rapid growth at higher $Re$ values, suggested a three-zone nonlinear model for flow in rough fractures. This three-zone model, relating effective hydraulic conductivity to $Re$, was also found to be appropriate for the simulation of water flow in the natural dolomite fracture. Increasing fracture roughness led to greater eddy volumes and lower effective hydraulic conductivities for the same $Re$ values.

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1. Introduction

Understanding fluid flow in rock fractures remains an open research question in the areas of contaminant hydrogeology, petroleum engineering and long-term disposal of nuclear waste. Rock fractures are a substantial contributor to fluid flow and solute transport in crystalline and sedimentary rock systems. The bulk flow characteristics along with secondary flow behavior are important factors affecting processes within these rough fractures.

Conventionally, bulk flow rates in fractures have been modeled as flow through an equivalent system of smooth parallel plates using the cubic law (Witherspoon et al., 1980) where flow is proportional to pressure gradient, with a proportionality constant, or transmissivity, related to the cube of the aperture. Using two-dimensional (2D) simulations of the Reynolds equation, Brown (1987) concluded that (i) the cubic law, with various measures of aperture, can approximate flow through synthetically generated fractures to within a factor of 2, (ii) the arithmetic average aperture gives better results than the other averages considered, and (iii) corrections to the cubic law accounting for tortuosity and contact area provide a better match to the Reynolds equation simulations. Zimmerman and Bodvarsson (1996) discussed the use of various simplifications to the Navier–Stokes equation including the lubrication equations and showed that at low Reynolds numbers ($Re < 1$), the effective cubic law aperture was lower than the actual aperture by a factor related to the ratio of the mean aperture to the aperture standard deviation. The authors concluded that this ratio, or the geometric mean of the aperture, in combination with a tortuosity correction factor, could effectively predict hydraulic conductivities. Oron and Berkowitz (1998) simulated flow in synthetic self-affine fractures with the Reynolds equation and showed that deviations from the local cubic law occur at contact ratios as low as 0.03–0.05 (Sisavath et al., 2003).

In experimental studies, using magnetic resonance imaging, Dijk et al. (1999) and Dijk and Berkowitz (1999) have found that the accuracy of the local cubic law depends strongly on the wall roughness, with sharp discontinuities in wall profile producing complex flow patterns. Experimental work by Plouraboué et al. (2000) in self-affine rough fractures with various translations of the opposing fracture surfaces indicated that heterogeneity in the flow field caused deviations from the parallel plate model for fracture flow. Méheust and Schmittbuhl (2003) observed anisotropic hydraulic behavior in experiments with rough fractures that had statistically isotropic heterogeneity in aperture (Boutt et al.,

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2006; Cardenas et al., 2009). Singh et al. (2015) examined fluid flow through granite fractures at very high fluid and confining pressures. They found that flow through the single granite fracture followed Darcy's law up to high fluid and confining pressures, but beyond a critical base pressure, flow changed from linear to nonlinear. Liu et al. (2016) also showed that in fracture networks, increasing the number of fracture intersections had a similar effect to increasing roughness with respect to the critical hydraulic gradient at which flow became nonlinear.

The effect of roughness on flow in fractures and validity of the local cubic law were examined by three-dimensional (3D) simulation of the Stokes and Navier–Stokes equations by Brush and Thomson (2003). They generated synthetic normally and lognormally distributed fracture aperture fields using exponential autocorrelation functions with varying correlation lengths. The authors concluded that deviations from the local cubic law were minimal for Re values less than unity. The authors also provided maximum criteria for local cubic law validity related to Re values and measures of fracture roughness (ratio of mean fracture aperture to correlation length or ratio of standard deviation in aperture to mean aperture).

Sjøt et al. (1999) simulated 2D flow in a single synthetic fracture (self-affine, Hurst exponent of 0.8) up to Reynolds numbers (Re) of 52. They also summarized previous literature in the area and identified three flow regimes: First, the vanishing inertia regime where Darcy's law is applicable; second, the weak inertia regime where the departure from Darcy's law is represented by a third-order correction (Mei and Auriault, 1991); finally, the strong inertia regime where the empirical Forchheimer relationship (Forchheimer, 1901) between hydraulic gradient and velocity has been shown to be applicable. The Forchheimer equation has a linear Darcy-like term with a Forchheimer permeability and a quadratic term with an inertial coefficient (Sjøt et al., 2000).

Bordier and Zimmer (2000), Cheng et al. (2008) and Moutsopoulos et al. (2009) showed that the Forchheimer and Izbash relationships provided a good fit to nonlinear flow in porous media, and George and Hansen (1992) showed that one form could be converted to the other subjected to maximum velocity limits. Chaudhary et al. (2011) fitted a power relationship between gradient and flow rate to model data for flow in idealized soil pores for Reynolds numbers from 0.1 to 1000, with a change in exponent between ranges of 0.1–10 and 10–1000. In experiments with sand-filled single fractures, Qian et al. (2011) showed an excellent fit between hydraulic gradients and discharge using both Forchheimer and Izbash methods. Bench scale experiments of fracture induced fluid and convection pressures, but beyond a critical base pressure, flow changed from linear to nonlinear. Liu et al. (2016) also showed that in fracture networks, increasing the number of fracture intersections had a similar effect to increasing roughness with respect to the critical hydraulic gradient at which flow became nonlinear.

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Chaudhary et al. (2011) simulated 2D flow in synthetic and natural fracture samples. In addition, wells that are under active pumping of water and convection pressures, but beyond a critical base pressure, flow changed from linear to nonlinear. Liu et al. (2016) also showed that in fracture networks, increasing the number of fracture intersections had a similar effect to increasing roughness with respect to the critical hydraulic gradient at which flow became nonlinear.

Sjøt et al. (1999) investigated the degree to which Re values and flow regime affected the development of flow along the fracture centerline in a rough fracture. The authors did not investigate the formation of eddies associated with increases in Re value in detail and used only one synthetic fracture. A number of studies have investigated the formation of eddies in idealized pore-and-throat geometries (Pozrikidis, 1987; Cao and Kitanidis, 1998; Bouquain et al., 2012).

Skjetne et al. (1999) investigated, through 2D modeling of the Navier–Stokes equations, the role of eddies in porous media and the reduction of hydraulic conductivity as eddies grew with increasing Reynolds number. They showed that eddies could exist in porous media at all scales of flow causing deviations from Darcy flow. Chaudhary et al. (2011) showed that flow in porous media over a wide range of Reynolds numbers would be best characterized by three zones of differing response of hydraulic conductivity to changes in Reynolds numbers. The first of these zones is where traditional low Reynolds simulations hold and can predict flow in a fracture; the second zone is where linearity breaks down and coincides with a rapid increase in eddy formation and growth; and the third zone is associated with a decrease in eddy growth rate, most likely associated with geometric constraints.

In fractured media, a rough surface rock fracture forms a system of abruptly changing channel widths that can create regions where secondary flows such as eddies can form (Qian et al., 2012). The results of Chaudhary et al. (2013) and Zou et al. (2015) suggested that fracture geometry, particularly roughness, significantly influences flow in fractures. In addition, wells that are under active development either for remediation or petroleum recovery processes may impose Reynolds numbers significantly higher than those typically found in natural groundwater systems. The current study is a systematic investigation of the effect of varying fracture roughness on flow in fractures over a wide range of Reynolds numbers, including application of the Izbash and Forchheimer models to the results. The investigation is conducted using the 2D general purpose graphical processing unit (GPGPU) based lattice Boltzmann method (LBM) of Briggs et al. (2014) to simulate water flow in synthetic and natural fracture samples.

2. Methods

2.1. Flow modeling

When complex geometries and varying Reynolds numbers are presented, a computational fluid dynamics (CFD) approach is required to capture the velocity distributions within a fracture (Dijk et al., 1999). Recently, the advances in computational efficiency have allowed the execution of CFD models on standard desktop computers and a number of commercially available finite volume software packages are available to address fluid flow problems in hydrogeology (Cardenas et al., 2007, 2009). Another CFD approach
is the LBM (Boult et al., 2006; Eker and Akin, 2006; Yan and Koplik, 2008) which is a group of methods for simulating fluid flow. LBM is based on the discrete Boltzmann equation from which the Navier–Stokes equations can be recovered using a Chapman–Enskog expansion (Succi, 2001). LBM intrinsically considers the unique boundaries of any given fluid regime and is used in this implementation at Reynolds numbers approaching 500.

Comprehensive documentation of the development of LBM can be found in the literature (Succi, 2001; Sukop and Thorne, 2005; Latt, 2007). For the purpose of describing laminar flow in a rock fracture, a 2D LBM was developed using nine velocity components and the Bhatnagar–Gross–Krook (BGK) collision approximation (Briggs et al., 2014). The two main components of LBM are the streaming and collision steps:

\[ f_n(x + v_n \Delta t, t + \Delta t) - f_n(x, t) = -\frac{1}{\tau} [f_n(x, t) - f_n^{eq}(x, t)] \]  

(1)

where the left-hand side of the equation represents the streaming step, and the right-hand side represents the collision step. The velocity distribution function, \( f \), represents the statistical movement of a fluid bundle along the nine velocity components, \( n \). Direction link \( e_n \) ensures that each fluid bundle moves a unit distance \( x \) at each time step \( t \). The relaxation parameter, \( \tau \), governs the rate at which the fluid tends towards equilibrium defined by \( f^{eq} \). For the LBM model, \( \tau \) also represents the kinematic viscosity of the simulated fluid and must be larger than 0.5 to represent physical fluids:

\[ \tau = 3\nu_l + 1/2 \]  

(2)

where \( \nu_l \) is the kinematic viscosity in lattice units. The model runs numerically (after Sukop and Thorne, 2005) to the velocity state, it compares well to the analytical solution with a relative average velocity error much less than 1% for Reynolds numbers up to 2008 which is a group of methods for simulating flow between parallel plates using incompressible fluids have been compared with analytical solutions. For laminar flow conditions, the Hagen–Poiseuille equation can be used to describe the horizontal velocity \( u \) through a cross-section:

\[ u(x) = \frac{G}{2\rho} (a^2 - x^2) \]  

(5)

This analytical solution yields a parabolic velocity profile where \( 2a \) is the slot width, \( x \) is the distance from the centerline, and \( G \) is the driving force. For the case of gravity-driven flow, \( G = \rho g \). The maximum velocity occurs at the centerline where \( x = 0 \) and the average velocity is \( 2/3 \) of the maximum velocity. Substituting these changes gives the driving force for the LBM:

\[ G = \frac{3\nu \bar{u}_{avg}}{a^2} \]  

(6)

where \( \bar{u}_{avg} \) is the average velocity.

Using the dimensionless Reynolds expression, physical parameters are converted to equivalent lattice parameters:

\[ Re = \frac{2\bar{u}_{avg} a}{v} \]  

(7)

Lattice spacing is determined by the geometry and discretization of the physical system. Lattice velocity is limited to a maximum of 0.1 lattice units per time step which arises from the approximations used in the LBM formulation to minimize compressibility effects (Sukop and Thorne, 2005). To ensure numerical stability, the relaxation parameter, \( \tau \), typically has a value of unity, however, it can be reduced to maintain the limit on lattice velocities for higher Reynolds numbers. Values of \( \tau \) approaching 0.5 do introduce numerical error into the simulation. However, as shown by Sukop et al. (2013), the numerical error is relatively small compared to the overall behavior of hydrogeological systems. The force of gravity in Eq. (6) is used in Eq. (4) to drive flow in the model. For the case of parallel plates, when the numerical model reaches steady state, it compares well to the analytical solution with a relative average velocity error much less than 1% for Reynolds numbers up to 500 and lattice spacing down to 5 units wide (normal to the bulk flow direction).

At higher flow rates (\( Re > 10 \)), porosity media and fractures, inertial effects will play an increasingly important role in flow behavior (Bear, 1972; Mei and Auriault, 1991; Skjetne and Auriault, 1999; Skjetne et al., 1999; Zimmerman et al., 2004) and the linear relationship between hydraulic gradient and flow rates (Darcy’s law) becomes nonlinear. A number of different empirical relationships have been used to describe the observed nonlinearity including the Forchheimer quadratic equation (Forchheimer, 1901) and Izbash’s power law relationship (Izbash, 1931). Forchheimer’s law is expressed as

\[ i = a_1q + bq^2 \]  

(8)

Similarly, Izbash’s relationship can be expressed as

\[ i = cq^\beta \]  

(9)

where \( i \) is the hydraulic gradient; \( a_1, b, c \) and \( \beta \) are the fitting coefficients; and \( q \) is the discharge rate. Analyses using nonlinear extensions to Darcy’s law are used to compare resulting fracture flow behavior at varying roughness and \( Re \) value.
2.3. Determination of effective hydraulic apertures in rough fractures

The local velocities from the LBM model were used to define an effective hydraulic aperture. Using the local velocity information and exact aperture distribution, flow conditions were calculated using the LBM. First, a gravity-driven flow cubic law is derived. Eq. (6) is rearranged for aperture:

\[ 2a^2 = \frac{6u_i u_{\text{avg}}}{g} \]  

(10)

The average velocity at any given cross-section is given by

\[ u_{\text{avg}} = \frac{Q}{2aW} \]  

(11)

where \( Q \) is the flow rate and \( W \) is the width of the fracture (kept at unity for the 2D case studied). Substituting Eq. (11) into Eq. (10) gives the equation for effective hydraulic aperture, \( 2a \):

\[ 2a = \left( \frac{12u_i Q}{gW} \right)^{1/3} \]  

(12)

Using the cubic law in this way, an effective hydraulic aperture is calculated using the flow rates from the LBM model. Each fracture is modeled using the LBM at Reynolds numbers of 0.01–500.

2.4. Fracture generation

A data set of fracture apertures was obtained for a dolomite rock sample approximately 350 mm long, 250 mm wide and 70 mm thick. The rock sample contained stylolites, which are planes of weakness, parallel to the length of the rock. A fracture was introduced in the rock block using the method described in Reitsma and Kueper (1994). Notches, 5 mm in size, were cut into two sides of the rock along a prominent stylolite. A load was applied to the notches using a uniaxial compression-loading machine until a fracture was developed along the stylolite. The remaining rock was trimmed to remove damaged zones, resulting in final dimensions of 280 mm × 210 mm × 70 mm (Fig. 1).

A 3D stereo-topometric measurement system, the Advanced Topometric Sensor (ATOS) II manufactured by GOM mbH, determined the surface profile of the fracture wall and its aperture distribution. For more details on the preparation of the sample and the ATOS II system, one can refer to Mondal and Sleep (2012, 2013) and Tatone and Grasselli (2009), respectively. A 16 mm 2D slice through the 3D surface created by the ATOS II was used in the LBM model and is shown in Fig. 2. Using a 2D approximation of the fracture to represent the 3D surface saves significant computational resources. A 2D system cannot capture or quantify the effects of contact points in a fracture and the impact of reducing effective apertures and increasing tortuosity (Zimmerman and Bodvarsson, 1996). Despite this, 2D modeling provides insights into the hydraulic behavior of fractures.

Fig. 1. Natural dolomite rock sample with fractures induced along existing stylolite. Sample length is 21 cm.

Fig. 2. Fracture profiles (b)–(j) generated using a synthetic fracture generator called SynFrac. Total fracture length is 100 mm and each fracture has a mean aperture of 1.7 mm, only the fractal dimension (FD) variable is changed in SynFrac. Fracture profile (a) represents a parallel plate system with an equivalent aperture of 1.7 mm. Fracture profile (j) represents a 16 mm long strip from a dolomite fracture with mean aperture of 0.1 mm.
fluid flow in rough fractures by allowing a high degree of spatial resolution at reasonable computational cost.

In addition to modeling flow in a segment of the dolomite rock fracture, flow was modeled in synthetic fractures. Synthetic fracture generation creates systems with controlled surface properties. To quantify the effects of surface roughness, a series of similar fractures with increasing roughness was generated with the software package SynFrac developed by Ogilvie et al. (2006). They expanded earlier work (Brown et al., 1995; Glover et al., 1998a,b) to capture the complex nature of natural fractures with synthetic approximations. Glover and Hayashi (1997) demonstrated that modeling a synthetic fracture at the centimeter scale applied directly to field flow measurements at the 100 m scale. An important consideration when generating synthetic fractures is capturing the fracture properties at all wavelengths. The top and bottom of a single fracture will have correlated geometry and surface properties at long wavelengths but are mostly independent at short wavelengths. The threshold separating long and short wavelengths is called the mismatch length. SynFrac has multiple methods for determining the mismatch length. In this study, the SynFrac implementation of Brown et al. (1995) mismatch length is set to 15 mm. Eker and Akin (2006) used SynFrac to generate fracture surfaces with mismatch lengths ranging from 5 mm to 25 mm, while Schwarz and Enzmann (2013) used SynFrac to generate fracture surfaces with mismatch lengths ranging from 10 mm to 30 mm.

In generating rough fracture surfaces, the desired fractal dimension or Hurst exponent must be specified. Bouchaud et al. (1990) found that fractures in aluminum alloys had a fractal dimension of 2.2 (Hurst exponent of 0.8). Schmittbuhl et al. (1993) found that a natural granite fault had a surface characterized by a Hurst exponent of 0.84. Boffa et al. (1998) measured Hurst exponents for granite and basalt fractures to be 0.8, while for sandstone fractures the Hurst exponent was in the order of 0.47 ± 0.05. Babadagli and Deveti (2003) found that fractal dimensions for laboratory-fractured rocks ranged from 2 to 2.7, with the highest values for sandstone. In using SynFrac to generate rough synthetic fracture surfaces, a range of fractal dimensions has been used. Eker and Akin (2006) used a fractal dimension range with SynFrac from 2.25 to 2.5 while Schwarz and Enzmann (2013) used a fractal dimension ranging from 2.05 to 2.5.

In the present study, the fractal dimension specified in SynFrac was varied between 2 and 2.35 (Table 1) consistent with the analysis of Ogilvie et al. (2006), developers of SynFrac who found that sandstone and granodiorite samples had fractal dimensions approaching 2.35. This fractal dimension, sometimes referred to as the box counting fractal dimension, corresponds to a range of Hurst exponents varying from 0.65 to 1.

Second, to analyze variations that may occur due to the pseudo-random number generator (SRNG) in SynFrac, multiple fractures with identical characteristic parameters were created while only varying the seeds of the Park and Miller SRNG algorithm. A 100 mm 2D profile was manually extracted from the data and selected such that it had no contact point. The arithmetic mean aperture of each fracture was kept constant (1.7 mm) for each study by manually adjusting the profile separation. Attention was also paid to the entry and exit of the fracture profile to ensure no interference with the periodic boundary conditions for fluid flow. Other SynFrac settings were kept constant including the resolution (1024 × 1024), standard deviation (1 mm) and anisotropy factor (1). The fracture length of 1024 elements is expanded to a grid length with 2048 elements using interpolation, resulting in a 48.8 µm element resolution.

The use of a fractal dimension for defining roughness is incomplete as fractal dimensions are not unique to an object, two similar but unique objects may have the same fractal dimension. It has also been shown that the direction of flow in a fracture yields varying results (Boult et al., 2006) whereas the fractal dimension of a surface is independent of the direction of measure. Some recent work (Tatone and Grasselli, 2009, 2010) has developed a roughness parameter used for measuring shear resistance in rock fractures based on angular thresholding of fracture surfaces. The concept of a shear based roughness translates well in fluid mechanics as wall shear stress compounded by the roughness of a fracture results in drag against the bulk flow. The roughness was calculated for each surface according to Tatone and Grasselli (2010), and then an average value was taken to represent both fractures with a single parameter.

### 3. Results and discussion

#### 3.1. Fracture flow

Fig. 3 shows a small (1 mm) segment of a 100 mm fracture with a Hurst exponent of 0.65 using the LBM model developed for this work. At low Reynolds number (Re = 0.01), some regions of the fracture show eddies that grow to occupy a significant portion of the system as the Reynolds number increases. Fig. 4 represents a 5 mm segment of the fracture where secondary flows such as eddies are evident and take the form of eddies or disconnected streamlines caused by eddies. The growth of eddies for sinusoidal pores is shown in Bouquin et al. (2012) for Re values up to 100 for a range of pore amplitudes and aspect ratios. At Re = 0.1 in a sinusoidal pore with an aspect ratio of 0.47 and a pore amplitude of 0.4, the smooth shape of the sinusoidal pore does not produce any noticeable eddies in the simulations of Bouquin et al. (2012) in contrast to the results for the fracture section shown in Fig. 3. From Fig. 4 it may be observed that the largest roughness features in the fracture walls have aspect ratios of approximately unity and amplitudes of approximately 0.15 for a Hurst exponent of 0.65. The eddies in the same sinusoidal pore of Bouquin et al. (2012) for a Re value of 10 occupy a much smaller fraction of the pore compared to the volume of the fracture roughness feature occupied by eddies at a Re value of 10 (Fig. 3).

Eddies can cause streamlines to detach from the bulk flow. The streamlines then re-attach at a location downstream depending on the geometry and Reynolds number (Armaly et al., 1983). The areas of detached flow reduce the effective hydraulic aperture, as they do not contribute to bulk flow.

Fig. 5 shows the relative effective hydraulic aperture (ratio of effective hydraulic aperture to the mean aperture). The results show that all fractures exhibit approximately constant effective aperture at Re < 1. At Re > 1, the effective aperture begins to decrease as Re increases. The rougher synthetic fractures, while having the same mean aperture, have smaller effective hydraulic apertures than that of a smooth fracture, indicating a larger fraction of the aperture contributing to secondary flows such as eddies. As

### Table 1

<table>
<thead>
<tr>
<th>Fracture type</th>
<th>3D fractal dimension</th>
<th>Hurst exponent, H</th>
<th>Angular threshold</th>
</tr>
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<tbody>
<tr>
<td>Synthetic fracture (using SynFrac)</td>
<td>2</td>
<td>1</td>
<td>9.62</td>
</tr>
<tr>
<td>2.05</td>
<td>0.95</td>
<td>10.72</td>
<td></td>
</tr>
<tr>
<td>2.1</td>
<td>0.9</td>
<td>12.41</td>
<td></td>
</tr>
<tr>
<td>2.15</td>
<td>0.85</td>
<td>14.43</td>
<td></td>
</tr>
<tr>
<td>2.2</td>
<td>0.8</td>
<td>16.73</td>
<td></td>
</tr>
<tr>
<td>2.25</td>
<td>0.75</td>
<td>19.79</td>
<td></td>
</tr>
<tr>
<td>2.3</td>
<td>0.7</td>
<td>23.15</td>
<td></td>
</tr>
<tr>
<td>2.35</td>
<td>0.65</td>
<td>27.29</td>
<td></td>
</tr>
<tr>
<td>Dolomite fracture</td>
<td>Not applicable</td>
<td></td>
<td>8.09</td>
</tr>
</tbody>
</table>
the Reynolds number increases, the rougher fractures show an increased rate of reduction of effective aperture compared to smoother fractures. Furthermore, the results show a gradual increase in roughness from Hurst exponents of 1 down to values of 0.65. From this transition, we capture the effect of secondary flow and the resulting effective hydraulic apertures. Similarly, Zou et al. (2015) found increasing complexity of eddy regions when the small-scale roughness features were included in their modeling compared to models of large-scale fracture roughness.

Previous studies in porous (Chaudhary et al., 2011) and fractured media (Zimmerman et al., 2004) have also shown a multi-zone behavior of hydraulic properties. Chaudhary et al. (2011) reported the transition beginning at Reynolds numbers around 1 for porous media. Skjetne et al. (1999) fitted the weak inertia equation over a Re range up to 0.1. The Re range from 1 to 25 was characterized as the transition regime from weak to strong inertia and the Forchheimer equation was fitted to Re values from 25 to 52. Zimmerman et al. (2004), from laboratory experiments and numerical simulations, found that the weak inertia regime was applicable in the Re range from 1 to 10, and the strong inertia regime was applicable for Re values above 20. Fourar et al. (2004) compared 2D and 3D pore-scale simulations of flow in periodic porous media, identifying Darcy, weak and strong inertia regimes and concluding that the weak inertia regime was significantly reduced in 3D simulations compared to that in 2D simulations.

As Reynolds numbers continue to increase, eddy growth is constrained by the increasing flow rates being driven through the fracture. Fig. 6 shows the rate of change of effective aperture with change in Re (slopes of curves in Fig. 5), similar to the reduction in flow tube diameter shown by Skjetne et al. (1999). The fracture flow regime can be divided into three zones, as done by Chaudhary et al. (2011), based on the rate of change of the effective aperture. In Zone I, there is little change of effective aperture as Re increases. In Zone II, the effective hydraulic aperture decreases at an increasing rate as Re increases. In Zone III, the effective hydraulic aperture increases at a decreasing rate as Re increases. The boundary between Zones II

Fig. 3. Flow streamlines in a fracture over a range of Reynolds number from 0.01 to 500. The fracture is a 2D slice of a 3D fracture generated in SynFracl with a Hurst exponent of 0.65. The segment shown has an overall dimension of approximately 1 mm × 1 mm.

Fig. 4. Simulated flow streamlines in a fracture at a Reynolds number of 500. The fracture is a 2D slice of a 3D fracture generated in SynFrac with a Hurst exponent of 0.65. The segment shown has an overall length of approximately 5 mm taken from the 100 mm long fracture simulated.

Fig. 5. Relative effective hydraulic apertures (ratio of effective hydraulic to mean apertures for each fracture) for the dolomite and synthetic fractures with varying roughness (given as a Hurst exponent, $H$).
and III is at approximately $Re = 30$ for the fractures generated by SynFrac and shown in Fig. 6. The dolomite fracture shows eddy growth at large Reynolds numbers, however, the dolomite fracture still shows a three-zone nonlinear effective hydraulic aperture relationship with Reynolds number.

Absolute results between SynFrac and the dolomite fracture show some variation possibly due to the differences in geometry and surface characteristics. Each synthetic fracture represents 100 mm of total length while the laboratory generated fracture is approximately 16 mm. Mean of the synthetic fracture aperture is 1.7 mm while the natural fracture is 0.1 mm. The surface characteristics were used in SynFrac without attempt to duplicate those of the dolomite fracture but rather characteristics that simplified numerical modeling. The dolomite fracture data show a rebound in eddy growth (Fig. 6) beginning at a Reynolds number of 50. The eddy growth rate would still be limited by fracture geometry and growth rates would slow down until the fluid transitions to a more turbulent regime.

At higher Reynolds numbers ($Re > 30$), in Zone III, the pressure drop in the synthetic fractures is nonlinearly related to the flow rate. In this higher Reynolds number regime, the Forchheimer equation can be used to describe the relationship between hydraulic gradient ($i$) and discharge rate ($q$ in m/s). Fig. 7 plots the smoothest and roughest fractures while the complete results are shown in Table 2. Fracture roughness affects both initial results for low $Re$ values as well as an increasing divergence from linearity at high roughnesses.

Similarly, the Izbash relationship can also be used to fit nonlinear flow regimes. Fig. 8 shows a linear region in Zones I and II and a change to a power law relationship in Zone III. The smoothest and roughest fractures are also plotted in Fig. 8 while Table 3 summarizes all roughnesses. The demarcation between Zones I and II and Zone III is located at the point of highest eddy growth rate previously shown to occur around $Re = 30$ for the synthetic fractures. The fracture roughness plays an additional role as the power law exponent in Zone III increases from 1.05 for the smoothest fracture up to 1.22 for the roughest fracture. This increase occurs with the growth of secondary flows in the fractures.

Chaudhary et al. (2011) found a power law exponent of 1.05 for slopes of effective aperture plots (Fig. 5) for the dolomite and synthetic fractures with varying roughness.

**Fig. 6.** Slope of effective aperture plots (Fig. 5) for the dolomite and synthetic fractures with varying roughness.

**Fig. 7.** Forchheimer fitting of discharge rates ($q$) for smooth ($H = 1$) and rough ($H = 0.65$) fractures at varying hydraulic gradients ($i$).

**Fig. 8.** Results of the Izbash power law fitting for nonlinear discharge rates ($q$) in fractures.

**Table 2** Comparison of Forchheimer coefficients.

<table>
<thead>
<tr>
<th>Hurst exponent</th>
<th>$a$</th>
<th>$b$</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>0.5</td>
<td>0.27</td>
</tr>
<tr>
<td>0.95</td>
<td>0.52</td>
<td>0.38</td>
</tr>
<tr>
<td>0.9</td>
<td>0.54</td>
<td>0.55</td>
</tr>
<tr>
<td>0.8</td>
<td>0.56</td>
<td>0.81</td>
</tr>
<tr>
<td>0.75</td>
<td>0.59</td>
<td>1.2</td>
</tr>
<tr>
<td>0.7</td>
<td>0.64</td>
<td>1.9</td>
</tr>
<tr>
<td>0.65</td>
<td>0.69</td>
<td>3.23</td>
</tr>
<tr>
<td>0.65</td>
<td>0.78</td>
<td>5.76</td>
</tr>
</tbody>
</table>

**Table 3** Comparison of Izbash power law constants and exponents.

<table>
<thead>
<tr>
<th>Hurst exponent</th>
<th>Zones I &amp; II</th>
<th>Zone III</th>
</tr>
</thead>
<tbody>
<tr>
<td>$c$</td>
<td>$\beta$</td>
<td>$c$</td>
</tr>
<tr>
<td>1</td>
<td>0.5</td>
<td>1</td>
</tr>
<tr>
<td>0.95</td>
<td>0.51</td>
<td>1</td>
</tr>
<tr>
<td>0.9</td>
<td>0.53</td>
<td>1</td>
</tr>
<tr>
<td>0.8</td>
<td>0.56</td>
<td>1</td>
</tr>
<tr>
<td>0.75</td>
<td>0.64</td>
<td>1</td>
</tr>
<tr>
<td>0.7</td>
<td>0.71</td>
<td>1</td>
</tr>
<tr>
<td>0.65</td>
<td>0.81</td>
<td>1</td>
</tr>
</tbody>
</table>
their pore-scale geometry at low \( Re \) (less than 10) and an exponent of 1.24 at higher \( Re \). The nonlinear behavior was also associated with the growth of eddies in their model.

The effective hydraulic aperture, calculated from the LBM results, is related to the region of the fracture contributing to the bulk flow (see results of Skjetne et al. (1999) for \( Re \) values up to 52 for an idealized fracture geometry) and is a fraction of the mean physical aperture as shown in Fig. 5. The remainder of the fracture, not contributing to bulk flow, defined as the eddy volume, contains complex flows, regions of streamline separation and eddy formation. The ratio of the bulk flow volume to the total fracture volume would be expected to be correlated to the ratio of the effective hydraulic aperture to the mean fracture aperture, while the ratio of eddy volume to total fracture volume would be related to 1 minus the ratio of the effective hydraulic aperture to the mean fracture aperture. The eddy volume ratios for all fractures as a function of \( Re \) are shown in Fig. 9. The eddy volume is similar to the ratio of eddy volume to the total volume in Chaudhary et al. (2011) and Bouquain et al. (2012) and the volume not included in the flow tubes of Skjetne et al. (1999).

The effective hydraulic aperture and resulting eddy volume are directly calculated from the LBM simulations and give insight into the relative effects of both roughness and Reynolds number. However, qualitatively visualizing the bulk flow and secondary flow paths within the fracture can help to understand the small-scale interactions that emerge as effective hydraulic behavior of the fracture. An estimate of the eddy and bulk flow regions can be determined locally using the overall eddy volume ratio to identify the threshold streamline that separates the bulk flow from the eddy volume. The nodes across any given section of the fracture at which the velocities drop below the product of the average velocity and the eddy volume ratio are found. An examination of flow features and eddies in fractures of varying roughness shows that these nodes across all cross-sections approximately demarcate the threshold streamline between bulk flow and secondary flows. Examples of the threshold, highlighted by thick red lines, are shown (Fig. 10) for a section of one synthetic fracture for a range of \( Re \) values. Calculation of the total eddy volume and eddy volume ratio using the threshold streamlines determined along the entire length of various fractures yields eddy volume ratios that are within a few percent of the values plotted in Fig. 9 that were determined from effective hydraulic apertures. For the smoothest fracture at the lowest Reynolds number (\( Re = 0.01 \)), the difference is 3.7% and reduces to 1.9% at \( Re = 500 \), with the streamline-based estimate being larger than the values plotted in Fig. 9 using the aperture values directly. For rougher fractures, the differences at a \( Re \) value of

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**Fig. 9.** Eddy volume ratio for the dolomite and synthetic fractures with varying roughness.

**Fig. 10.** Flow streamlines (black lines with arrows) and the eddy volume that does not contribute to bulk flow (thick red line). Cross-section shown represents approximately 1.8 mm\(^2\) from a segment of a SynFrac cross-section with an original Hurst exponent of 0.65.
0.01 are approximately 10% for the roughest fracture. However, as Reynolds number increases, the difference approaches 1% or less for all fractures.

At lower $Re$, the threshold streamline closely follows the fracture surface. However, even at the lowest Reynolds numbers, complex fracture surfaces introduce boundary layer effects that cause deviations relative to flow calculated for an equivalent parallel plate system. At higher $Re$, the effective hydraulic aperture decreases and the streamline showing secondary flows straightens and moves away from the surface. The fracture surfaces act as a series of backward facing steps with many overlapping detachment and re-attachment locations. Flow in the regions associated with eddies is considered to be a negligible contribution to total fracture flow relative to bulk flow; however, its proximity to the boundary is important for many engineering problems such as solute transport and biofilm development.

To examine the variation of results for fractures with the same statistical characteristics, five different SynFrac fractures were created with SRNG with the same statistical properties but with different seeds (Fig. 11). Results show some variations as expected, however, the overall behavior is consistent with the three-zone model presented earlier.

### 3.2. Tortuosity

Using the local velocity simulated by the LBM, a tortuosity value was calculated using the actual flow path in the fracture. Brown et al. (1998) defined tortuosity as the ratio of actual fluid path to the total projected length of the fracture. Crandall et al. (2010) used advective particle tracking to average the fluid path of over a hundred simulated particles. When the entire velocity profile of the fracture is known, a more detailed approach can be used that traces the actual path of the fastest moving fluid streamline and determines its length which is divided by the actual fracture length to calculate tortuosity (Skjetne et al., 1999). The fastest streamline is assumed to represent the natural tortuosity of the bulk flow. The path of fluid streamlines changes as seen in Figs. 3 and 9 due to both roughness and Reynolds numbers. The results in Fig. 12 show a trend of increasing tortuosity with increasing roughness similar to that reported in previous work (Tsang, 1984; Brown, 1989; Crandall et al., 2010).

The dependence of tortuosity on the Reynolds number is more complex and CFD approaches are required to make this determination. Initially, flow paths are determined by the geometry, or roughness, of the system. Then, as Reynolds number increases, eddies form and grow in regions of abrupt aperture change perturbing existing streamlines and in turn increasing tortuosity. The complex interaction leads to a nonlinear relationship between Reynolds number and tortuosity (Fig. 12). General behavior follows a three-zone trend similar to the effective hydraulic aperture. Zone I is constant at $Re < 1$ with a transition to a nonlinear relationship in Zones II and III. The replicate synthetic fractures (Fig. 13) show a more pronounced shift from Zone II to Zone III as tortuosity increases significantly. Although the eddy growth rate in Zone III is reduced, eddies are at their largest and could explain the significant increase at the highest Reynolds number.

### 3.3. Directionality

A measure of roughness was chosen that could account for any directional anisotropy in the fracture. For Reynolds numbers less than 100, the vast majority of groundwater flows, flow rates in the fractures generated by SynFrac showed less than 1% variation when reversing flow direction. The random creation of fracture surfaces in SynFrac does not seem to create directionally dependent fractures with the default program settings as roughness was also varied by approximately 1% (for the same SynFrac fracture between the forward and reverse directions). Directional dependence becomes a factor when large-scale fracture features are present causing differentiation in flow streamlines. Large backward facing steps would be an example of a geometry creating directionally sensitive results.
4. Conclusions

Lattice Boltzmann simulations of flow in a natural dolomite fracture and in several synthetic fractures with increasing roughness were conducted. Emphasis was placed on the effect of roughness on secondary flows as well as bulk fluid flow. It was found that eddies formed beginning at a Reynolds number around unity and experienced significant growth as Re was increased. This is a similar range to previous work (Zimmerman et al., 2004), however, it is the complex flow arising at the boundaries, such as eddies, that are directly associated with the change in effective hydraulic aperture. This eddy growth behavior suggests a three-zone nonlinear model of fracture flow similar to that found for porous media by Chaudhary et al. (2011) and for fractures by several authors including Skjetne et al. (1999) and Zimmerman et al. (2004). This work expands the application of the three-zone model to fractures over a range of roughnesses (Hurst exponents). In Zone I at Re < 1, effective aperture is constant but dependent on initial fracture geometry; Zone II begins at Re approaching 1 where conventional fracture modeling breaks down as a result of the significant increase in eddy growth rates. The reduction in eddy growth rate represents the boundary of Zones II and III and can vary for the fracture system being modeled. The nonlinear Zone III can be effectively described by extensions of Darcy’s law using the Izhbash relationship while the Forchheimer relationship can describe flow over the entire Re range examined. For smooth fractures and Re < 30, discharge is linearly related to gradient but with different offsets for increasing roughness. At Re > 30, discharge is nonlinearly related to gradient with increasing Izhbash and Forchheimer coefficients for increasing roughness.


Conflict of interest

The authors wish to confirm that there are no known conflicts of interest associated with this publication and there has been no significant financial support for this work that could have influenced its outcome.

References


Dr. Scott Briggs is a post-doctoral fellow at the University of Toronto. His current work focuses on the numerical modeling of sulphide diffusion in bentonite with applications for the long-term storage of nuclear waste. He obtained his doctorate in Environmental Engineering from the University of Toronto with a focus on contaminant hydrogeology. His PhD research included modeling the impact of single fracture roughness on the flow, transport and development of biofilms.