Investigation of Gravity-Driven Infiltration Instabilities in Smooth and Rough Fractures Using a Pairwise-Force Smoothed Particle Hydrodynamics Model

Elena Shigorina,* Alexandre M. Tartakovsky, and Jannes Kordilla

This work investigates small-scale infiltration dynamics in smooth and rough single fractures using a three-dimensional multiphase pairwise-force smoothed particle hydrodynamics (PF-SPH) model. Gravity-driven infiltration instabilities in fractures under unsaturated conditions can significantly influence the arrival time of tracers or contaminants, and the rapid and localized recharge dynamics in fractured–porous aquifer systems. Here, we study the influence of roughness and injection rate on fluid flow modes and flow velocity. Three types of fractures are considered with different degrees of roughness, including a smooth fracture. Both the rough and smooth fractures exhibit flow instabilities, fingering, and intermittent flow regimes for low infiltration rates. In agreement with theoretical predictions, a flat fluid front is achieved when the flux $q$ supplied to a fracture is larger than the gravitationally driven saturated flux $q > k \rho g/\mu \cos(\varphi)$, where $k$ is the intrinsic permeability of the fracture, $\rho$ is a density, $\mu$ is the viscosity, and $\varphi$ is the fracture inclination angle measured from the vertical direction. To characterize the flow instability, we calculate standard deviations of velocity along the fracture width. For the considered infiltration rates, we find that an increase in roughness decreases the flow velocity and increases the standard deviation of velocity. This is caused by a higher likelihood of flow discontinuities in the form of fingering and/or snapping rivulets. To validate our unsaturated flow simulations in fractures, we estimate the scaling of specific discharge with normalized finger velocity, compute the relationship between fingertip length and scaled finger velocity, and find good agreement with experimental results.

Abbreviations: DFN, discrete fracture network; PF, pairwise-force; SPH, smoothed particle hydrodynamics.

Special Section: Nonuniform Flow across Vadose Zone Scales

Core Ideas
• We study infiltration dynamics in smooth and rough fractures using a 3D SPH model.
• Roughness induces the formation of flow fingering and preferential flow paths.
• Fractal roughness leads to a deceleration of average fingertip velocities.
• The velocity variance of fingers positively correlates with the degree of roughness.
• Normalized finger velocity and length scale in accordance with analytical predictions.

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of large-scale problems (e.g., the regional hydraulics of fault zones) (Eker and Akin, 2006; Hendricks and Flury, 2001).

Most numerical large-scale studies use the Richards’ equation (Richards, 1931) to describe partially saturated flow in fractured media, which is treated as a porous continuum (Heiweil et al., 2015; Therrien and Sudicky, 1996). In the presence of a porous matrix, multi-continuum approaches can be used to resolve the large ratio of fractures and porous matrix permeabilities (Kordilla et al., 2012; Wang and Narasimhan, 1985; Wu et al., 2004).

In fully saturated systems, the parallel plate model (Dershowitz and Einstein, 1988; Snow, 1996) allows for a better discrete representation of internal fracture flow dynamics, which are subject to ongoing modifications to account for roughness effects (Wang et al., 2015).

However, in partially saturated fractures, the distribution of water within the fracture depends on matric potential (of the adjacent porous medium), local aperture, and flow-rate-dependent flow modes (droplets and slugs, rivulets, films), which influence the formation of instabilities (fingering) and hence the travel times. Furthermore, the fracture-specific water distribution to a large degree controls the inter-fracture partitioning and redistribution dynamics (Jones et al., 2018; Kordilla et al., 2017; Noffz et al., 2018), which is of importance for the application in discrete fracture network models (DFN; Cacas et al., 1990; Hyman et al., 2015). The complexity of unsaturated flows and the existence of several highly dynamic flow regimes in fractures have been demonstrated by various authors (Ghezzehei, 2004; Tokunaga and Wan, 1997, 2001). Depending on infiltration rates, flow regimes switch from adsorbed films (with average flow velocities on the order of $10^{-7} \text{ m s}^{-1}$) to droplet flows and finally rivulet flows at high infiltration rates. Finally, at very high flow rates, rivulets merge and continuous (wavy) films can occur.

Transitions between flow modes and, therefore, the instability of an injected fluid front depend on the complex force balance between gravity, capillary, and viscous forces. Even under idealized conditions (e.g., smooth fracture surfaces and constant infiltration rates), fluid fronts in fractures are prone to develop instabilities (i.e., fracture-specific preferential flow paths) due to the strong impact of gravitational forces and relatively low capillary action (Nicholl et al., 1994). The number of these discontinuities (rivulets and/or droplet streams) is generally larger in rough fractures (Wang et al., 2016; Briggs et al., 2017). Injected fluid follows the paths of least resistance, accumulates in depressions, or flows around elevated parts of the rough surface to form fracture-specific preferential flow pathways.

Laboratory experiments can provide valuable insights into infiltration dynamics in unsaturated fractures. Most laboratory setups investigating unsaturated flows consist of two (textured) parallel glass plates (Hele–Shaw cell), separated by a small aperture, representing a fracture (Jones et al., 2018; Nicholl and Glass, 2005; Nicholl et al., 1999). This allows visual observation of the internal transient flow dynamics (i.e., the propagation of the fluid). Laboratory experiments in natural fractures are challenging. For example, flow in a natural fracture was considered by Nicholl et al. (1994), where only the post-infiltration state could be analyzed after the setup was disassembled. Laboratory studies of saturated flow have, for example, been performed by Li et al. (2018), who used cement casts to create surfaces based on fractal roughness and obtained information about flow channeling effects by measuring outflow rates along the fracture width. Brown et al. (1998) used rubber molds to manufacture transparent epoxy replicas of natural fractures and measured flow velocities using nuclear magnetic resonance imaging. They found that flow velocities in the fracture plane may vary by several orders of magnitude, and maximum velocities may be higher than the mean flow velocity by a factor of five.

Of direct relevance to our present work are the studies of Nicholl et al. (1994) and Nicholl and Glass (2005), who experimentally studied the finger formation across a wide range of flow rates and fracture inclinations as a function of the gravitational and viscous pressure differentials along infiltrating fingers.

In this work, we investigate the development of fluid front instability and formation of complex flow modes in smooth and rough individual fractures by using an efficient three-dimensional parallelized pairwise-force smoothed particle hydrodynamics (PF-SPH) model implemented in LAMMPS (Plimpton, 1995; Kordilla et al., 2017). The PF-SPH–LAMMPS code has been extensively validated (Kordilla et al., 2013, 2017; Shigorina et al., 2017) and used to simulate highly intermittent, gravity-driven, free-surface flows under dynamic wetting conditions. Our recent work (Kordilla et al., 2013; Shigorina et al., 2017) investigated the effect of surface roughness on droplet and rivulet flows. Here, we study the effect of roughness on average flow velocity and fluid flow profile in fractures.

We use the PF-SPH model to characterize fluid front instabilities in smooth and rough fractures for various infiltration rates in terms of finger front velocity. We observe transitions between flow modes and fluid flow profiles for different infiltration rates. Flow in fractures with two types of surface roughness are studied and compared with flow dynamics in a smooth fracture. For each infiltration rate, the average flow velocity is measured. We use the standard deviation of flow velocity to quantify flow instability or degree of dispersion and compare the standard deviation for different infiltration rates and degrees of roughness. Finally, we study the specific discharge scaling with the normalized finger velocity and the relation between fingertip length and scaled finger velocity and find good agreement with the experimental results of Nicholl and Glass (2005).

 Governing Equations and the PF-SPH Method

We assume that free-surface flow of water in a fracture can be described by the continuity equation

$$\frac{\partial \rho}{\partial t} = -\rho (\nabla \mathbf{v}). \quad x \in \Omega_\tau (t)$$

[1]
and the momentum conservation equation
\[
\frac{d\mathbf{v}}{dt} = -\frac{1}{\rho} \nabla P + \frac{\mu}{\rho} \nabla^2 \mathbf{v} + \mathbf{g}, \quad x \in \Omega_t (t)
\]  
subject to the Young–Laplace boundary condition
\[
P n = \tau_w n + S \sigma n, \quad x \in \partial \Omega_{wa}
\]  
and the continuity condition at the water–air interface \( \partial \Omega_{wa} \)
\[
(\mathbf{v} - \mathbf{v}_b) n = 0, \quad x \in \partial \Omega_{wa}
\]
where \( \rho \) is a density, \( t \) is a time, \( x \) is any variable of the domain \( \Omega_0 \), \( \sigma \) is the surface tension of water, and \( \tau_w \) is a viscous stress tensor along the water–air–solid contact line \( S \).

The contact angle is prescribed at the water–air–solid contact line and the no-slip boundary condition at the boundary between water and solid phases. Here, \( \tau_w = |\mu (\nabla \mathbf{v} + \nabla \mathbf{v}^T)| \) is the viscous stress tensor, \( \mathbf{v} \) is the fluid velocity, \( \mathbf{v}_b \) is the boundary velocity, \( P \) is the pressure, \( \mu \) the viscosity, \( \mathbf{n} \) is the normal vector pointing away from the nonwetting phase, and \( \mathbf{g} \) the gravitational acceleration.

To numerically solve the governing equations, we extend the domain \( \Omega_t (t) \) occupied by water to include the solid phase (walls of the fractures) as \( \Omega_t (t) = \Omega_t (0) \cup \Omega_s \), where \( \Omega_t \) is the extension of \( \Omega_t (0) \). Next, we discretize \( \Omega_t (0) \) with “fluid” particles with positions denoted by \( \mathbf{r}_j \in \Omega_t (0) \) and \( \Omega_s \) with solid particles with positions \( \mathbf{r}_j \in \Omega_s \). The positions of solid particles are fixed and their velocities are set to zero. The positions and velocities of fluid particles are found from the momentum conservation equation discretized with the weakly compressible pairwise SPH scheme (Kordilla et al., 2013, 2017; Morris et al., 1997; Tartakovsky and Meakin, 2005a):
\[
\frac{d\mathbf{v}_j}{dt} = -\sum_{j=1}^{N} \left[ \frac{p_j}{\rho_j} \mathbf{r}_j \right]_{r_j} dW \left( r_j, b \right) \mathbf{dr}_j +2\mu \sum_{j=1}^{N} \left[ \frac{\rho_j \rho_j}{\rho_j} \mathbf{v}_j \right]_{r_j} dW \left( r_j, b \right) \mathbf{dr}_j + \frac{1}{\rho_j} \sum_{j=1}^{N} \mathbf{F}_{ij}, \quad \mathbf{r}_j \in \Omega_t (t)
\]  
and
\[
\frac{d\mathbf{r}_j}{dt} = \mathbf{v}_j, \quad \mathbf{r}_j \in \Omega_t (t)
\]
where the summation is performed on all particles including fluid and solid particles. Here, \( \mathbf{r}_j = \mathbf{r} - \mathbf{r}_j \) and \( r_j = |\mathbf{r} - \mathbf{r}_j| \), \( m_j = m \) is the (constant) mass of particle \( j \), \( \rho_j \) and \( P_j \) are the density and pressure of fluid carried by particle \( j \), \( b \) is the support range of the kernel \( W \), \( \mathbf{v}_j \) is a velocity, \( \mathbf{F}_{ij} \) is an interaction force between particles \( i \) and \( j \), and \( N \) is a total number of particles in the domain. Fluid and solid particles are assumed to have the same mass and \( \rho_j \) is computed for both fluid and solid particles as (Morris et al., 1997; Tartakovsky and Meakin, 2005a)
\[
\rho_j = \sum_{j=1}^{N} m_j W \left( r_j, b \right), \quad \mathbf{r}_j \in \Omega_t (t) \cup \Omega_s
\]
This expression conserves mass exactly and, therefore, can be used instead of the mass conservation (continuity) Eq. [1]. The pressure of both fluid and solid particles is computed from the equations of state Batchelor (1967):
\[
P_i = P_0 \left[ \frac{\rho_i}{\rho_0} \right] ^{\gamma} - 1, \quad \mathbf{r}_j \in \Omega_t (t) \cup \Omega_s
\]
where
\[
P_0 = \frac{c^2 \rho_0}{\gamma}
\]
\( \gamma = 7, \rho_0 \) is the equilibrium particle density, and the speed of sound \( c \) is chosen such that the relative density fluctuation \( |\rho - \rho_0|/\rho \) is small (<3%) to approximate an incompressible fluid.

The weighting function \( W \) is modeled with the third-order Wendland function (Wendland, 1995):
\[
W \left( r_j, b \right) = \alpha_4 \left[ 1 - \frac{r_j}{b} \right] ^3 \left[ 4 \frac{r_j}{b} - 1 \right] ^2 \text{ if } 0 \leq r_j < b
\]
\[
W \left( r_j, b \right) = \frac{1}{4} \left[ 2 - \frac{r_j}{b} \right] ^3 \text{ if } r_j \geq b
\]
where \( \alpha_4 = 21/(2\pi b^3) \).

The force \( F_{ij} \) in Eq. [5] is used to impose the Young–Laplace boundary condition (Tartakovsky and Panchenko, 2016). Following Tartakovsky and Meakin (2005a), Tartakovsky and Panchenko (2016), and Kordilla et al. (2013), we use a combination of kernel functions to generate a continuous function with short-range repulsive and long-range attractive components:
\[
F_{ij} = s_{ij} \left[ A W \left( r_j, b_1 \right) \frac{r_j}{r_{ij}} + B W \left( r_j, b_2 \right) \frac{r_j}{r_{ij}} \right] \text{ if } r_j \leq b
\]
\[
F_{ij} = 0 \text{ if } r_j > b
\]
where \( W \) is the cubic spline function
\[
W \left( r_j, b \right) = \left[ 1 - \frac{3}{2} \frac{r_j}{b} \right] ^2 \left[ \frac{3}{4} \frac{r_j}{b} \right] ^3 \text{ if } 0 \leq \frac{r_j}{b} < 0.5
\]
\[
W \left( r_j, b \right) = \left[ \frac{1}{4} \left[ 2 - \frac{r_j}{b} \right] ^3 \text{ if } 0.5 \leq \frac{r_j}{b} < 1
\]
\[
W \left( r_j, b \right) = 0 \text{ if } \frac{r_j}{b} \geq 1
\]
where \( A, B, b_1, \) and \( b_2 \) determine the shape of \( F_{ij} \). We set \( A = 8, B = -1, b_1 = 0.5, \) and \( b_2 = 1 \). For a given \( F_{ij} \) shape, \( s_{ij} \) determines the magnitude of the surface tension and static contact angle.

The parameter \( s_{ij} \) is equal to \( s_{ij} \) for the interaction between two fluid particles and \( s_{ij} \) for the interaction between fluid and solid particles. The ratio of \( s_{ij} \) and \( s_{ij} \) controls the static and dynamic contact angles. For a liquid to wet the surface, \( s_{ij} \) should be set greater than \( s_{ij} \) and vice versa.

In SPH, the no-slip boundary condition at the fluid–solid boundary can be imposed by using ghost particles that mirror
fluid particles in the direction normal to the nominal solid interface (Liberstsky et al., 1993) or uniformly distributed particles in the solid phase (i.e., in the fracture wall; Morris et al., 1997; Zhu et al., 1999). These methods require determining the ratio of normal distances from fluid and mirror particles to the nominal solid boundary (the proximity ratio), which becomes challenging for highly irregular surfaces. Moreover, the computational costs of these methods are high compared with simpler bounce-back conditions, as demonstrated by Tartakovsky and Meakin (2006), Tartakovsky et al. (2009), and Kordilla et al. (2013, 2017).

To enforce the no-slip boundary condition at the nominal fluid–solid interface, we use the proximity ratio (Holmes et al., 2011). We first define the state of a particle (i.e., fluid or solid) with ψ and χ. Next, a phase-specific number density \( n^s_i \) is calculated to easily determine the solid–fluid boundary even for highly irregular (rough) surfaces:

\[
n^s_{i,\psi} = \sum_{j=1}^N \delta_{\psi,\chi} W(r_{i,\psi} - r_{i,\chi}, b)
\]

where the Kronecker delta is

\[
\delta_{\psi,\chi} = \begin{cases} 
1 & \psi = \chi \\
0 & \psi \neq \chi 
\end{cases}
\]

The proximity ratio for a fluid particle can then be obtained as

\[
\phi_f = \frac{n^s_i}{n_i}
\]

where \( n_i \) is the (total) particle density \( n_i = \rho_i/m_i \) defined as

\[
n_i = \sum_{j=1}^N W(r_i - r_j, b)
\]

The value of \( \psi \) varies from 1 for particles in the fluid phase at a distance greater than \( h \) from the fluid–solid interface to 0.5 at the interface to zero for particles in the solid phase at a normal distance greater than \( h \). Note that for \( m_j = m \), the total particle number density can be found as \( n_i = \rho_i/m_i \). To enforce a no-slip boundary condition, we return fluid particles along the normal back into the flow domain once they penetrate the boundary (i.e., for \( \phi_f < 0.5 \)). A smoothed color function \( c_i \) is used to obtain the normals:

\[
c_i = \sum_{j \in \Omega_F} \frac{m_j}{\rho_j} W(r_{ij}, b)
\]

where the above summation is only on fluid particles. The surface normals can then be calculated from the gradient

\[
\hat{s}_i = \nabla c_i
\]

Penetrating particles have their velocities inverted and are returned along the normal direction by a distance \( \Delta d \) proportional to the proximity ratio:

\[
\Delta d = \omega \Delta x \left( 1 - \frac{\phi_f}{0.5} \right)
\]

In this work, we set \( \omega = 1 \), which we found to prevent particle penetration even for very complex surface geometries, and \( \Delta x \) is a particle spacing. In most cases, the pressure gradient and interaction force are sufficient to prevent the penetration of fluid particles in the solid phase.

Equation [5] is integrated with a modified velocity-Verlet time-stepping scheme (Ganzenmüller et al., 2011):

\[
v_i(t + \Delta t) = v_i(t) + \frac{1}{2} a_i(t)
\]

\[
v_i(t + \Delta t) = v_i(t) + \Delta t a_i
\]

\[
r_i(t + \Delta t) = r_i(t) + \Delta t v_i(t) + \frac{1}{2} \Delta t^2 a_i
\]

\[
v_i(t + \Delta t) = v_i(t) + \frac{1}{2} \Delta t a_i(t + \Delta t)
\]

Once new positions \( r_i(t + \Delta t) \) are calculated, the new particle acceleration \( a_i(t + \Delta t) \) can be obtained using an extrapolated velocity \( v_i \). To ensure stability of the numerical solution, the following time step constraints are satisfied (Tartakovsky and Meakin, 2005a):

\[
\Delta t \leq \frac{0.25 b}{3c}
\]

\[
\Delta t \leq 0.25 \min \left( \frac{b}{3|a_j|} \right)^{3/2}
\]

\[
\Delta \leq \min \left( \frac{b}{3|a_j|} \right)^{3/2}
\]

where \( |a_j| \) is the magnitude of acceleration \( a_j \).

Gravity-Driven Flow Instability in Initially Dry Fractures

Infiltration into a fracture is controlled by gravity, viscous, and capillary forces. When gravitational forces dominate, the flow becomes unstable, and fingering occurs. Instability of the gravity-driven fluid front occurs when the flux \( q \) supplied to a fracture is less than the gravitationally driven saturated flux \( K_s \cos(\varphi) \) (Nicholl et al., 1994):

\[
q < K_s \cos(\varphi)
\]

where \( K_s \) is the saturated hydraulic conductivity

\[
K_s = \frac{k \sin (\varphi)}{\mu}
\]

\( k \) represents the intrinsic permeability of the fracture, and \( \varphi \) is the fracture inclination angle measured from the vertical direction.

In this work, we numerically study the propagation of a fluid front in smooth and rough fracture planes along with the
dependence on the supplied flux. Specifically, we investigate the dynamic switching of flow regimes between droplets, rivulets, and films and how it controls the formation of instabilities and average arrival times.

Flow in Smooth Vertical Fractures

In the section below, we model flow between two smooth parallel vertical surfaces with dimensions 10 by 30 cm separated by a 2.0-mm gap (Fig. 1, left). Fluid particles are assigned a density and viscosity of water \( \rho_f = 1000 \text{ kg m}^{-3} \) and \( \mu = 1.296 \times 10^{-3} \text{ Pa s} \), respectively. The equilibrium density of solid and fluid particles is set to 1000 kg m\(^{-3}\). Initially, the SPH particles (solid and fluid) are placed on a uniform cubic lattice with spacing \( \Delta x = 2 \times 10^{-4} \text{ m} \), which results in a fluid particle mass of \( m = \rho_0 \Delta x^3 = 8 \times 10^{-9} \text{ kg} \). The mass of individual solid particles is set to \( m \). The speed of sound is \( c = 2.5 \text{ m s}^{-1} \), the gravitational acceleration \( g = 9.81 \text{ m s}^{-2} \), and the smoothing length is set to \( h = N^{1/3} \Delta x = 6.84 \times 10^{-4} \text{ m} \). Here, \( N = 40 \) is the number of particles within a volume \( h^3 \), which was found to be sufficient for three-dimensional simulations including the effect of surface tension and is related to the number density \( n = N/h^3 \). The fluid is injected at the fracture top with constant volumetric flux \( Q \). According to Eq. \[22\], for a stable fluid front to develop, the flux must be \( Q \geq 5.06 \times 10^{-4} \text{ m}^3 \text{ s}^{-1} \) \((q > 2.52 \text{ m}^3 \text{ s}^{-1})\). To investigate the fluid front instability, we perform simulations with \( Q \) varying from \( Q \) to \( 8 \times 10^{-4} \text{ m}^3 \text{ s}^{-1} \) (Fig. 2). For this simulation setup, the fracture is discretized with 2,250,000 solid particles, and the fluid is discretized with 670,000 to 14,900,000 particles, depending on the infiltration rate and duration. Simulations are run on 64 and 128 processors.

To measure the average flow velocity, we divide the fracture surface into \( n = 20 \) longitudinal sections of equal width. Each section has a width of 0.5 cm and length of 30 cm. At every time step, we measure the fluid front propagation within each section. The fluid velocity for each section \( v_{\text{sec}} \) is found as

\[
v_{\text{sec}} = \frac{z(t + \Delta t) - z(t)}{\Delta t}
\]

where \( z(t + \Delta t) \) and \( z(t) \) are the maximum fluid front positions into the direction of flow at time step \((t + \Delta t)\) and \(t\), respectively. The average flow velocity \( \bar{v} \) for the whole fracture is then found as an arithmetic mean of flow velocities within each section:

\[
\bar{v} = \frac{1}{20} \sum_{i=1}^{20} v_{\text{sec}}
\]

The velocities \( \bar{v} \) for different \( Q \) values are listed in Table 1. The average velocity \( \bar{v} \) (superscript \( s \) denotes the smooth fracture) increases with increasing \( Q \) (Fig. 3, squares).

Figure 2 shows the fluid distributions inside a smooth fracture for different infiltration rates and the transition between flow regimes. For fluxes up to \( Q > 1 \times 10^{-5} \text{ m}^3 \text{ s}^{-1} \), the flow mainly consists of droplets, partially leaving behind trailing films. At fluxes \( Q > 1 \times 10^{-5} \text{ m}^3 \text{ s}^{-1} \), the flow transitions into a rivulet-dominated regime with occasional occurrence of snapping droplets and/or rivulets. Similar flow regimes were observed in our previous SPH studies (Kordilla et al., 2013, 2017). In this work, we extend our studies to observe a transition between rivulets and film flow. For higher flow rates, \( Q > 4 \times 10^{-5} \text{ m}^3 \text{ s}^{-1} \), we observe the formation of snapping films, which extend throughout the periodic boundaries on the lateral sides of the domain. Finally, a stable fluid front develops for \( Q > 5.06 \times 10^{-4} \text{ m}^3 \text{ s}^{-1} \) (Fig. 2f) in accordance with the theoretical condition (Eq. \[22\]).

To quantify the instability of the fluid front, we calculate the standard deviation \( s \) of velocity within each section \( v_{\text{sec}} \) with respect to the mean flow velocity \( \bar{v} \) (Table 1). Squares in Fig. 4 show the standard deviations in smooth fractures for each infiltration rate. The largest \( s = 0.0813 \) is observed for \( Q = 8 \times 10^{-6} \text{ m}^3 \text{ s}^{-1} \). For \( Q \geq 8 \times 10^{-6} \text{ m}^3 \text{ s}^{-1} \), the standard deviation decreases and reaches its minimum value \( s = 0.002 \) when a stable fluid front is developed at \( Q = 5.06 \times 10^{-4} \text{ m}^3 \text{ s}^{-1} \).
For $Q > 5.06 \times 10^{-4}$ m$^3$ s$^{-1}$, the standard deviation remains equal to its minimum value.

**Flow in Rough Vertical Fractures**

Fractures encountered in geological environments have rough surfaces, despite the fact that they are often approximated as smooth in, for example, discrete fracture network modeling (Hyman et al., 2015; Therrien and Sudicky, 1996). In our previous work using the PF-SPH model (Kordilla et al., 2013, 2017; Shigorina et al., 2017), we investigated various effects of surface roughness on droplet flow and wetting dynamics, including capillary-Bond number scaling functions, onset of trailing film formation, relation of microscale and macroscopic hydrophobic–hydrophilic behavior for Cassie and Wenzel droplets, and the effect of roughness anisotropy on droplet flows. In this work, we extend these studies to investigate the effect of roughness on the behavior of highly complex flows with flow regimes ranging from droplet to droplet-to-rivulet and rivulet-to-film flows.

Following Tartakovsky and Meakin (2005b) and Kordilla et al. (2013), we create rough fractures characterized by the Hurst exponent $z$ (Bouchaud et al., 1990) and an initial maximum value $D$ for the random displacement from a planar surface. It was shown that $z$ often assumes values of $0.8 \pm 0.05$ for consolidated impermeable rocks (Bouchaud, 1997; Ponson et al., 2006); however, wider ranges of $0 < z < 0.09$ have been measured as well (Boffa et al., 1998; Sahimi, 2011).

For our simulations, we created two rough fractures with dimensions 10 by 30 cm, $z = 0.75$, and $D = 10.0$ and 20.0 mm. The fracture aperture is $b = 2.0$ mm. Figure 1 (middle and right) shows the fractures used, where light colors represent elevated parts of the height field and dark colors are associated with depressions.

**Table 1. Statistical properties for various fluxes ($Q$) in smooth and rough fractures.**

<table>
<thead>
<tr>
<th>$Q$ (m$^3$/s)</th>
<th>Smooth†</th>
<th>Rough‡</th>
<th>$\bar{v}$</th>
<th>$\bar{v}_{10}$</th>
<th>$\bar{v}$</th>
<th>$\bar{v}_{20}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>4 \times 10^{-6}</td>
<td>0.15</td>
<td>0.0346</td>
<td>0.13</td>
<td>0.368</td>
<td>0.12</td>
<td>0.387</td>
</tr>
<tr>
<td>8 \times 10^{-6}</td>
<td>0.25</td>
<td>0.0813</td>
<td>0.21</td>
<td>0.0927</td>
<td>0.23</td>
<td>0.0956</td>
</tr>
<tr>
<td>2 \times 10^{-5}</td>
<td>0.41</td>
<td>0.0291</td>
<td>0.36</td>
<td>0.0433</td>
<td>0.32</td>
<td>0.0477</td>
</tr>
<tr>
<td>4 \times 10^{-5}</td>
<td>0.55</td>
<td>0.0154</td>
<td>0.50</td>
<td>0.251</td>
<td>0.43</td>
<td>0.0339</td>
</tr>
<tr>
<td>6 \times 10^{-5}</td>
<td>0.69</td>
<td>0.0035</td>
<td>0.61</td>
<td>0.0047</td>
<td>0.53</td>
<td>0.0075</td>
</tr>
<tr>
<td>1 \times 10^{-4}</td>
<td>0.89</td>
<td>0.0023</td>
<td>0.71</td>
<td>0.0036</td>
<td>0.65</td>
<td>0.0061</td>
</tr>
<tr>
<td>3 \times 10^{-4}</td>
<td>1.63</td>
<td>0.0021</td>
<td>1.55</td>
<td>0.0033</td>
<td>1.45</td>
<td>0.0039</td>
</tr>
<tr>
<td>5 \times 10^{-4}</td>
<td>2.53</td>
<td>0.0020</td>
<td>2.50</td>
<td>0.0030</td>
<td>2.41</td>
<td>0.0032</td>
</tr>
<tr>
<td>8 \times 10^{-4}</td>
<td>3.69</td>
<td>0.0020</td>
<td>3.60</td>
<td>0.0030</td>
<td>3.50</td>
<td>0.0031</td>
</tr>
</tbody>
</table>

† $\bar{v}$ (m/s), average flow velocity in smooth fractures; $\bar{v}_s$, standard velocity deviation in smooth fractures.
‡ $\bar{v}_{10}$ (m/s), average flow velocity in rough fractures with $\Delta = 10$ mm; $\bar{v}_{20}$, standard velocity deviation in rough fractures with $\Delta = 20$ mm; $\bar{v}_{10}$, average flow velocity in rough fractures with $\Delta = 10$ mm; $\bar{v}_{20}$, standard velocity deviation in rough fractures with $\Delta = 20$ mm.
Table 1 summarizes the velocities and standard deviation values (Nicholl and Glass, 2005, Fig. 27). To compare this experiment with our simulations, we calculate the specific discharge
\[ q = \frac{Q}{bd} \]  
and the normalized velocity \[ v_{\Delta=10,20}^{*,f} = \frac{v_{\Delta=10,20}^{*,f}}{b} \] 
where \( d \) is the fracture width, \( v_{\Delta=10,20}^{*,f} \) is the normalized averaged flow velocity from simulations, the superscripts \( s,r,f \) represent smooth, rough, and simulation fractures, respectively, and \( v_{f}^{*} \) is the normalized velocity of individual fingers from experiments. The experimental and simulation data are listed in Table 2.

Figure 7 shows \( v_{f}^{*} \) as a function of \( q \). On the logarithmic plot, \( \log(v_{f}^{*}) \) shows linear dependence on \( \log(q) \) that assumes the power law dependence \( v^{*} = q^{p} \). A similar power law dependence was observed in the experiments with \( p = 0.48 \). In our simulations, the exponent \( p \) lies in the range between 0.50 and 0.55 for smooth and rough fractures, which is close to the experimental value of \( p \) (Fig. 7).

Next, we investigate fingertip length \( L_{\text{tip}} \) as a function of fingertip velocity and compare our simulation results with an analytical solution and experimental data from Nicholl and Glass (2005, Fig. 30). Here, the term fingertip is often also referred to as elongated droplets or slugs. For the sake of completeness, the following is an excerpt from Nicholl and Glass (2005). For a stagnant fingertip, the viscous forces vanish and capillary forces balance the gravitational component, i.e.,
\[ \Delta P_{g} - \Delta P_{c} = 0 \]  
where gravitational forces are approximated as
\[ \Delta P_{g} \approx \Delta \rho g \cos(\varphi) y_{g}^{f} \] 

Table 2. Comparison of experimental (Nicholl and Glass, 2005, Fig. 27) and simulation data.

<table>
<thead>
<tr>
<th>Experiment†</th>
<th>Simulation‡</th>
</tr>
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<tbody>
<tr>
<td>( q )</td>
<td>( v_{f}^{*} )</td>
</tr>
<tr>
<td>1.7 \times 10^{-5}</td>
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<td>3.7 \times 10^{-5}</td>
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<td>59.1</td>
</tr>
<tr>
<td>2.46 \times 10^{-3}</td>
<td>81.3</td>
</tr>
</tbody>
</table>

† \( q \) (m/s), specific discharge; \( v_{f}^{*} \) (1/s), normalized velocity of individual fingers.
‡ \( v_{f}^{*} \) (1/s), normalized velocity for smooth fractures; \( v_{f=10}^{*} \) (1/s), normalized velocity for rough fractures with \( \Delta = 10 \) mm; \( v_{f=20}^{*} \) (1/s), normalized velocity for rough fractures with \( \Delta = 20 \) mm.
and act over a characteristic length scale $h_g$. The pressure differential within the water phase of a fingertip is approximated as

$$\Delta P \approx \sigma \left[ \frac{1}{r_1} + \frac{1}{r_2} \right]_{\text{front}} - \left[ \frac{1}{r_1} + \frac{1}{r_2} \right]_{\text{trail}}$$

[30]

where the radius of curvature $r_1$ (the first principal radius spanning both walls of the fracture) and the in-plane curvature $r_2$ at each point could not be determined in the laboratory experiments. To estimate the fingertip length $L_{\text{tip}}$ from Eq. [28] together with Eq. [29] and [30], Nicholl and Glass (2005) assume that the pressure along the leading and trailing edge can be approximated by the wetting and draining pressure head ($\psi_w$ and $\psi_d$) such that

$$L_{\text{tip}} = \frac{\psi_w - \psi_d}{\cos(\varphi)}$$

[31]

Further, they found that for a vertical fracture ($\cos(\varphi) = 1$), the measured stagnant fingertip lengths are very close to the values obtained from Eq. [31]. Hence, for our simulations, we define

$$\psi_w - \psi_d = T_{\text{tip}}$$

[32]

where $T_{\text{tip}}$ is the average length of stagnant fingertips found to be 1.0 cm in our simulations.

Under dynamic conditions, viscous forces are introduced into the force balance, which now becomes

$$\Delta P_g - \Delta P_v - \Delta P_r = 0$$

[33]

Viscous forces act over a characteristic length scale $h_v$ and are approximated by

$$\Delta P_r \approx \eta \mu h_v (kk_r)^{-1}$$

[34]

where $k_r = 1$ under the assumption that fingertips are fully saturated and $\nu$ is the fingertip velocity. Insertion of Eq. [29], [30], and [34] into Eq. [33] and assuming the characteristic length scales correspond to the fingertip length (i.e., $L_{\text{tip}} = h_g = h_v$), the following expression for the fingertip length is obtained:

$$L_{\text{tip}} = \frac{\psi_w - \psi_d}{\cos(\varphi) \left( 1 - \frac{\nu}{K_s k_r \cos(\varphi)} \right)^{-1} T_{\text{tip}} \left( 1 - \frac{\nu}{K_s} \right)^{-1}}$$

[35]

Because the wetting pressure is dependent on the fingertip velocity, the above equation can only serve as a first-order approximation. Nicholl and Glass (2005) found a better fit to their data using the expression

$$L_{\text{tip}} = \frac{\psi_w (1 - \dot{\nu}^2) - \psi_d}{(1 - \nu^2) \cos(\varphi)}$$

[36]

which takes into account the dependence of the leading contact angle (related to the dynamic wetting pressure $\psi_w$) on velocity, where $\epsilon = 0.1$ is an empirical coefficient.

Figure 8 shows the simulation data and experimental results of Nicholl and Glass (2005) (Fig. 30 therein), as well as the analytical solutions Eq. [35] and [36] for the scaled fingertip length $[L_{\text{tip}} \cos(\varphi)]$ as a function of scaled fingertip velocity $\dot{\nu} = \nu//K_k k \cos(\varphi)$. The analytical solution Eq. [35] shows a good fit with simulation data for $T_{\text{tip}} = (\psi_w - \psi_d) 1.0$ cm and $\epsilon = 0.1$. Similar to Nicholl and Glass (2005), we also observe greater discrepancies between the analytical solution and the simulations results for intermediate values of the scaled velocity $\dot{\nu}$.

**Discussion**

In our previous work (Shigorina et al., 2017), we observed that, depending on its geometry and orientation, a “structured” surface roughness can accelerate or decelerate flow. In this work, we create
random rough fracture surfaces with $\zeta = 0.75$ and $\Delta = 10.0$ and 20.0 mm, to approximate natural rough fracture surfaces. Our simulation results show that with increasing $\Delta$, the velocity $\bar{v}$ decreases for all infiltration rates (Fig. 3, Table 1). For a given infiltration rate, the average velocity $\bar{v}$ in rough fractures can be 1.4 times lower than $\bar{v}$ in the smooth fracture.

Here, we demonstrate the influence of fracture roughness and viscous and capillary forces on flow instability. Our simulations show that even in a smooth fracture, fluid flow is unstable for $Q < 5 \times 10^{-5} \text{m}^3 \text{s}^{-1}$ (Fig. 2a–2c). For $Q$ between $5 \times 10^{-5}$ and $5 \times 10^{-4} \text{m}^3 \text{s}^{-1}$, the evolving fluid front appears stable (straight) (Fig. 2d and 2e). However, because of fluid snapping and merging, the fluid flow velocities may significantly fluctuate.

For the rough fractures, the fluid front is unstable for $Q < 5 \times 10^{-4} \text{m}^3 \text{s}^{-1}$ (Fig. 5a–5c and 6a–6c). For $Q > 5 \times 10^{-4} \text{m}^3 \text{s}^{-1}$, the fluid front is stable for both rough and smooth fractures, and the velocity $\bar{v}$ is constant (Fig. 2f, 5f, and 6f).

To characterize the instability, we calculate standard deviations of flow velocity $s$ (Fig. 4, Table 1). Unstable flows are characterized by rivulets (or fingering flow) and/or droplet streams in parts of the fracture, whereas the remaining fracture is dry with flow velocities close to zero. We observe a peak of standard deviation for a discharge $Q = 8 \times 10^{-6} \text{m}^3 \text{s}^{-1}$ (Fig. 4). At a discharge $Q = 8 \times 10^{-6} \text{m}^3 \text{s}^{-1}$, ~50% of the fracture is saturated (exhibiting high flow velocities), and 50% of the fracture is dry with very low velocity or no flow occurring. Hence, the distribution of flow velocities gives rise to the highest standard velocity deviation relative to the mean flow velocity. According to Eq. [22] and in accordance with our results for fluxes approaching $Q = 5.04 \times 10^{-4} \text{m}^3 \text{s}^{-1}$, the standard deviation of velocity decreases as the number of instabilities (i.e., rivulets or droplet pathways) decreases, hence the likelihood of localized preferential flow paths declines. For flows $Q < 8 \times 10^{-6} \text{m}^3 \text{s}^{-1}$, the standard deviation decreases again as the number of individual streams approaches a maximum (this has, for example, been studied by Ghezzehei [2005] using an energy-minimization principle for free-surface systems), and therefore the (bulk) system exhibits a more diffuse behavior again. It should be noted that for even lower injection rates (that we have not studied in this work), the flow may even be bounded by only one side of the fracture such that slugs (i.e., droplets bounded by both fracture walls) may be transformed into “true” droplets, and for even lower flow rates, thin films bounded by only one side of the fracture wall may occur. This transition has been studied, for example, by Ghezzehei (2005) and is most likely characterized by a different behavior of the velocity standard deviation. Our results show that with increasing $\Delta$, the standard deviation $s$ increases for all infiltration rates due to the increasing likelihood of finger and droplet stream formation. Fluid front instabilities create preferential flow pathways, which affects the fracture–matrix interaction area, wetting dynamics, infiltration processes, and arrival times of tracers or contaminants in the vadose zone.

However, in fully saturated smooth and rough fractures, the standard deviation $s$ reaches its minimum value. As expected, in the fully saturated fractures, the mean flow velocity $\bar{v}$ is equal to the infiltration rate.

Comparison of our simulation with the experiments of Nicholl and Glass (2005) shows good agreement for two of the main characteristics of the experimental setup. Despite the differences in geometry (our fractures are smaller, but with larger aperture), the scaling of normalized velocities with specific discharge shows similar trends, and the scaling of fingertip length with scaled velocity agrees with the analytical predictions.

In our simulations, the scaling of normalized velocities $v_{\Delta, s}^{\zeta, \bar{v}}$ and specific discharge, $v^* \sim q^*$, yields exponents on the order of 0.5 to 0.55 (the exponent is increasing with increasing roughness) compared with $p = 0.48$ in the laboratory experiments. The simulations cover a slightly greater range of normalized velocities; however, extrapolated normalized velocities for the given scaling exponents (Fig. 7) and lower velocity ranges are expected to be below the experimental ones. The main reason for this is that flow velocities from the simulations are averaged along the whole fracture, whereas in the experiment, only velocities of individual rapid fingers were measured.

The comparison of fingertip length and scaled fingertip velocities between experiments and simulations proves that the model is able to represent the complex case of a gravity-driven instability. The values of $L_{\text{tip}}$ for the experiment are larger than the simulated ones. This is mainly caused by the wider aperture used in the simulations, which triggers faster snapping of rivulets due to the increase of gravitational force compared with the capillary component; hence, the resulting fingers are smaller.

**Conclusion**

In this work, we used a three-dimensional PF-SPH model to simulate gravity-driven flow in smooth and rough fractures. Two types of rough fractures with $\zeta = 0.75$ and $\Delta = 10.0$ and 20.0 mm were considered.

To study the effect of fracture roughness on the front instability and flow regimes, the fluid was injected in fractures with a constant flux, and the average flow velocity and standard deviation were computed for different infiltration rates.

Our results indicated that the flow velocity in smooth and rough fractures increases with an increasing infiltration rate. We observe the transition between flow regimes, which has been validated in our earlier studies via laboratory and numerical experiments (Kordilla et al., 2017). For both smooth and rough fractures, the rivulet flow regime is dominant for $Q \leq 4 \times 10^{-5} \text{m}^3 \text{s}^{-1}$, whereas for higher fluxes, a snapping or continuous film was observed. For the smooth fracture, the fluid front remained stable for $Q > 4 \times 10^{-5} \text{m}^3 \text{s}^{-1}$, whereas for rough fractures, the fluid film front formed some preferential pathways. For the fluxes $Q > 5 \times 10^{-4} \text{m}^3 \text{s}^{-1}$, the whole fracture filled with water, and the fluid profile was stable for rough and smooth fractures. Furthermore, we observed deceleration of flow velocity due to roughness. Average velocities $\bar{v}$ in rough
fractures were smaller than the corresponding velocities \( v^s \) in smooth fractures.

Our results show that the largest standard velocity deviation \( s \) (a measure of front instability) occurs for \( Q = 8 \times 10^{-6} \text{ m}^3 \text{ s}^{-1} \) in both the smooth and the rough fractures. For \( Q > 8 \times 10^{-6} \text{ m}^3 \text{ s}^{-1} \), the standard deviation decreases and reaches its minimum value when a stable fluid front develops. Because of the roughness inducing flow channeling effects, for a given \( Q \), the standard deviation \( s^r \) in rough fractures was larger than \( s \) in smooth fractures.

The analysis of flux-dependent fluid flow velocity and instability in smooth and rough vertical fractures is required to gain a better understanding of the formation of preferential flow paths. Because of their flow-focusing properties, such fractures not only contribute to the fracture-specific flow path but are important to understand large-scale hydro(geo)logical problems (i.e., infiltration and percolation through whole fracture networks and associated processes, such as aquifer recharge or contaminant transport [vulnerability]). Large-scale fracture networks and connections between fractures induce a variety of additional partitioning and dispersion processes. Preferential flow paths along fracture networks exhibit depth-dependent reshaping of the flow and input signal due to flow rate specific partitioning dynamics at fracture intersections (Kordilla et al., 2017), and hence, understanding the distribution of flow within each fracture is an important factor in defining the partitioning dynamics for fracture cascades and networks (Noffz et al., 2018).

For saturated systems promising extension of the classical cubic law are applied, for example, to create two-dimensional depth-averaged representations of complex three-dimensional flows via dimension reduction in individual fractures (Modified Local Cubic Law; Wang et al., 2015). Unsaturated flows in fractures exhibit an even higher degree of internal complexity and to bridge the gap between large-scale applications (e.g., DFN models) and small-scale process-oriented models of unsaturated flows in fractures. Further developments and studies are required to enhance existing solutions (Dippenaar and Van Rooy, 2016).

Convergence of large-scale applications and process-oriented models may also be facilitated by an increase in numerical efficiency and/or computing power. Nonuniform resolution (or adaptivity) in SPH is not yet well established and has been defined as one of the most important goals within the SPH community. Adaptive resolutions in principle only require particle-dependent sizes of \( h \) (and modifications of the kernel computation when particles of different size interact) to account for variable particle number densities (volumes). This is rather straightforward for static grids (e.g., mesh-based approaches) and solid SPH boundarys but becomes challenging once highly dynamic fluid interfaces in the Lagrangian framework are considered. To apply nonuniform resolution to such flows, adaptive splitting and coalescence schemes are required and consequently a set of splitting–coalescence conditions, which are challenging to define for free-surface flows in the presence of surface tension.

Despite methodological advances (e.g., dynamic nonuniform resolution) and increases in computing power, the simulation of unsaturated flows through whole fracture networks (field scales with millions or billions of fractures in three dimensions) is not possible in the near future with any numerical method that discretizes the Navier–Stokes equation. On fracture scales, computational costs are largely affected by the highly anisotropic properties with respect to the resolved length scales. In-plane dimensions of fractures are generally orders of magnitude larger (centimeters to meters) than aperture widths (micrometers to millimeters), which consequently control the resolution required to discretize the flow field along the fracture normals, as well as the height-dependent roughness field. Vertically depth-integrated approaches such as the modified local cubic law model (Wang et al., 2015) are computationally more efficient; however, they fail to resolve saturated and unsaturated flow processes in the presence of preferential flow paths, which may induce strong hydraulic contrasts, especially for wide aperture fractures. Here, free-surface flows, that is, flows bounded by only one fracture surface, may occur and hence invalidate or limit the application of vertically depth-integrated modeling approaches.

For now, the outcomes of such discrete simulations presented in this paper can only serve as a tool to identify the importance of individual fracture-scale processes and inter-fracture partitioning dynamics to enhance DFN models or even upscaled lumped parameter models (Liu et al., 2003, 1998).

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