

Tracer dispersion in two-dimensional rough fractures

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Tracer diffusion and hydrodynamic dispersion in two-dimensional fractures with self-affine roughness are studied by analytic and numerical methods. Numerical simulations were performed via the lattice-Boltzmann approach, using a boundary condition for tracer particles that improves the accuracy of the method. The reduction in the diffusive transport, due to the fractal geometry of the fracture surfaces, is analyzed for different fracture apertures. In the limit of small aperture fluctuations we derive the correction to the diffusive coefficient in terms of the tortuosity, which accounts for the irregular geometry of the fractures. Dispersion is studied when the two fracture surfaces are simply displaced normally to the mean fracture plane and when there is a lateral shift as well. Numerical results are analyzed using the Λ parameter, related to convective transport within the fracture, and simple arguments based on lubrication approximation. At very low Péclet number, in the case where fracture surfaces are laterally shifted, we show using several different methods that convective transport reduces dispersion.

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I. INTRODUCTION

Tracer spreading in flows between parallel walls has received considerable attention since the celebrated work of Taylor [1]. This problem is of fundamental importance in a variety of fields and, in particular, transport processes through artificial or natural porous media. In general, the dispersion of a tracer carried along by a flowing fluid in a medium of disordered structure, such as hydrocarbon or water reservoirs, involves a combination of convection and dispersion through the microscopic pore space of the rock itself and through macroscopic channels such as fractures. In the simplest case of Poiseuille flow in a Hele-Shaw cell, which in several applications is used to model fractures [2–5], the vanishing velocity near the solid gives rise to a large dispersion, quadratic in the Péclet number [1,6]. However, one frequently encounters systems in which the channel aperture varies along the flow direction or in which the channel walls have some rugosity. This is the case for fractured rocks, in which fractured boundaries can be usually described as correlated, self-affine fractals [7]. The roughness exponent is usually found to be close to 0.8 and to be insensitive to the material and to the fracturing process [8–10]. Most of the studies dealing with varying channel aperture model the fluctuations as slowly varying periodic functions [11]. Only a few works deal with more realistic models of fractures, such as random rugosities perpendicular to the flow [12] or self-affine fractures [13,14].

In the present paper we present numerical simulations of tracer diffusion and dispersion in self-affine fractures. The simulations are two dimensional and the fluid flow and tracer spreading are computed using the lattice-Boltzmann (LB) method. We will first discuss, in Sec. II, the implementation of the LB method to simulate diffusive transport. We shall propose a boundary condition which improves the accuracy and validity of the method, particularly when describing narrow fractures. In Sec. III we will evaluate this boundary condition against previous ones in two different cases: Diffusion (Sec. III A) and Taylor dispersion (Sec. III B) in a two-dimensional straight channel.

After reviewing some basic facts about self-affine surfaces (Sec. IV), we investigate, in Sec. V, how the complex geometry of fracture surfaces affects the diffusive transport (zero mean flow velocity). We also study the dependence of diffusivity on the size of the gap between complementary fracture surfaces. We will show that it is possible to derive an analytic expression, which accounts for the geometric effects on the diffusivity, in the limiting case where the roughness associated with the fracture surface is small compared to the mean aperture.

In Sec. VI we study dispersive transport in two different situations: first, when the two surfaces are simply displaced normally to the mean fracture plane. In this case, we will show that a description in terms of a parameter Λ , related to *dynamically connected* pore space, accounts for a large part of the dispersion enhancement due to low-velocity zones in the fracture channel. Second, we show that when there is a lateral shift as well as a normal displacement, an increase in dispersion is obtained. Finally, we present a result showing that dispersion is diminished in the presence of convection at low Péclet numbers. This effect is found when the surfaces are shifted and the convective transport is weak enough.

II. LATTICE-BOLTZMANN MODEL WITH THE BGK COLLISION OPERATOR

Our goal is to study various aspects of transport in fractures which are sensitive to the fracture roughness. Since we consider convection and dispersion in a highly irregular geometry, the lattice-Boltzmann method [15–17] is particularly convenient. In this algorithm, fictitious particles move between neighboring sites on a lattice, with suitable collision rules, and the boundary of the flow domain is simply a surface of sites where boundary condition rules should be imposed. We use a version of the LB model first proposed by Qian *et al.* [18], with a cubic lattice in 3 dimensions and 19 velocities (D3Q19 in the terminology of [18]). The collision operator is approximated by a single relaxation parameter λ ,

the Bhatnagar-Gross-Krook (BGK) model [19], and the local equilibrium distribution given in [18] is used. This pseudo-equilibrium distribution locally preserves mass and momentum values, and is formulated specifically to recover the Navier-Stokes equation at large length and time scales. As usual, we use the lattice spacing as the unit length and the time step in the simulations as the unit time. In the following, quantities will be measured in terms of the lattice spacing and simulation time step. Note that, since we are concerned with incompressible flows, we do not need to introduce a dimension of mass.

The model used for miscible fluids is a straightforward extension of the model restricted to describe simple fluids. Following the convention of Rothman and Zaleski [16], we will distinguish between particle types by assuming that the particles are colored. The pseudo equilibrium color distribution given in [16] is used, and a single relaxation parameter λ_D (BGK approximation) is used in the equation that describes the advection and diffusion of color. In addition to mass and momentum, color is also a conserved quantity.

The basic variables of the model are the distribution functions N_i , corresponding to the mean occupation number of particles in the direction i at a given node, and Δ_i , describing the relative amount of color [20]. Since the evolution of the total population is independent of the color of the particles, the hydrodynamic equations for mass and momentum may be obtained as in the simple fluid case. In other words, the time evolution of the N_i 's is independent of the Δ_i 's. These evolution equations are then coupled to the evolution of color, through the local fluid velocity. Thus, the diffusive behavior of the fluids is superimposed on the underlying Navier-Stokes dynamics.

The fact that the information on mass density and flow is decoupled from the information on color opens the possibility of imposing different boundary conditions (BC's) on the populations describing fluid flow (N_i) and those describing advective-diffusive transport (Δ_i). Specifically, for a nonslip BC on the solid surface, we shall use the simplest implementation of particle exclusion—the bounce-back rule (BB), where the particles incident on the boundary are propagated back into the directions from which they came. On the other hand, for color concentration a different macroscopic BC is desired, i.e., a zero color gradient normal to the solid surface.

Diffusion boundary conditions

As mentioned, we will study tracer dispersion in narrow gaps between self-affine solid surfaces. Thus, in this situation, the BC's imposed at the solid surfaces becomes a crucial aspect of the simulation method.

In previous works concerning lattice BGK models for miscible fluids, BC's imposed on color concentration at solid boundary were not distinguished from those used to simulate fluid flow. In these situations, the relevance of the BC at solid surfaces varies depending on the particular system under consideration. In some cases, when simulating bulk processes, as in [20,21], there is no need to treat the BC separately, and periodic boundary conditions on all distribution functions may be used. In other cases, fully three-

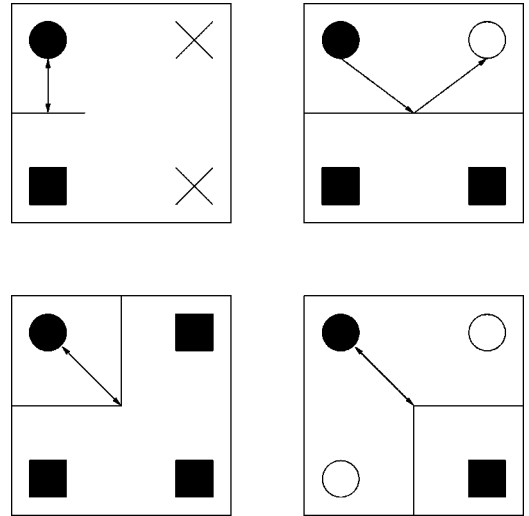


FIG. 1. Schematic view of the bounce-forward collision rule. Solid squares represent solid sites, open circles represent fluid sites, and solid circles represent particles. Solid lines correspond to the fluid-solid interface, situated halfway between solid and fluid sites. Arrow lines represent incoming and outgoing trajectories.

dimensional problems in Helle-Shaw cells are described in terms of the two-dimensional LB model by the modification of the forcing to account for the viscous drag of the top and bottom plates of the cell [22–24]. Therefore, molecular diffusion in the transverse direction is not described and similar BC's can be applied to all fields. In the others, where fluid flows in complex geometries [13] or in narrow channels bounded by solid surfaces [25,26], the above-mentioned distinction in BC's would be desirable.

Here we will use a different set of BC's for color concentration to ensure a zero color gradient normal to the solid surface. To this end, we implement a mirror-reflection condition or bounce-forward (BF) rule, where upon collision only the normal component of the particle velocity is changed. In Fig. 1 we show a schematic view of the BF collision rule. The last case was chosen arbitrarily, due to its very simple implementation, among the different possibilities that satisfy the mirror-reflection-type condition. For instance, it would be also consistent to split the incoming concentration into the two neighboring sites.

Physically, BB has the (approximate) effect of making both components of the fluid velocity vanish at the solid, consistent with the nonslip condition. A passive tracer may, however, diffuse along a solid boundary, so the relevant condition is that only the normal component of the flux vanish at a solid. The bounce-forward rule is the obvious LB realization of the physical boundary condition.

To answer the question whether this BC improves the LB method for miscible fluids we shall present the results of numerical simulations using both BB and BF in two different situations: diffusion and Taylor hydrodynamic dispersion in a two-dimensional straight channel.

III. COMPARISON BETWEEN BB AND BF RULES: NUMERICAL SIMULATIONS

We will exhibit a comparison between BB and BF, in two applications, diffusion and Taylor dispersion in a two-

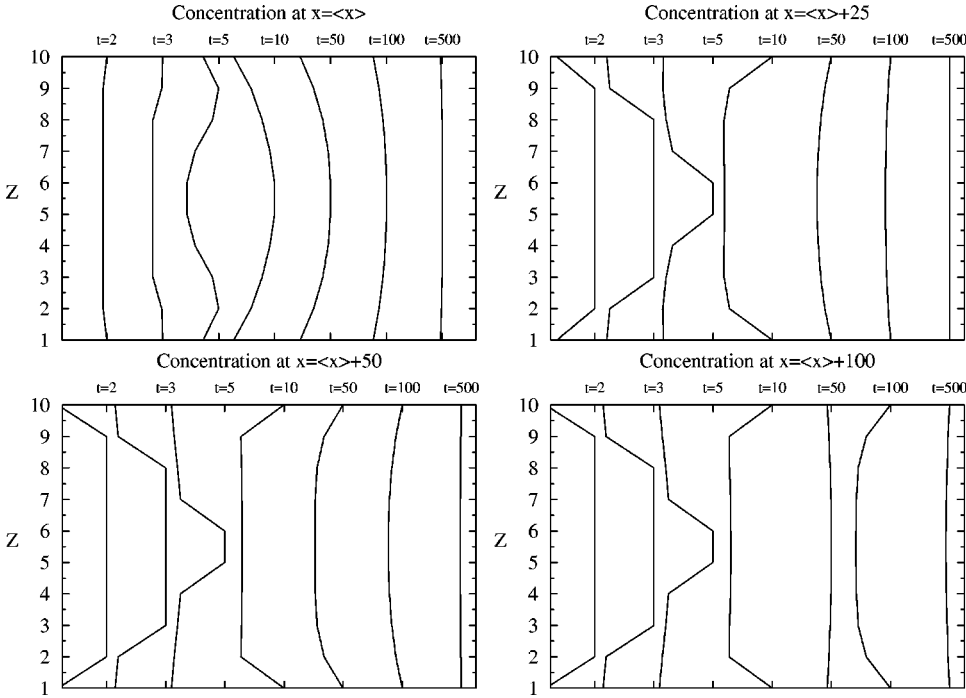


FIG. 2. Vertical dependence of the color concentration. Horizontal axes represent normalized concentration. For clarity the curves corresponding to different times are shifted horizontally by a constant value. Results correspond to numerical simulations in a channel of width $H=10$ and length $L=512$. The initial condition is a Gaussian color distribution centered at $x=256$ and with $\sigma^2=4.0$. The relaxation parameter is $\lambda_D=0.2$ corresponding to a bulk diffusion coefficient $D_m=1.5$.

dimensional channel. These situations are particularly important in terms of addressing the validity and accuracy of the above-mentioned boundary conditions, particularly if one is interested in further use of them in complex geometries.

A. Diffusion in a two-dimensional straight channel

Diffusion was studied varying the channel width H from 4 to 40 in grid sites, in a channel of length $L=512$, with periodic BC's used at both ends. In the LB model the diffusion coefficient in bulk is given by

$$D_m = \frac{1}{3} \left(\frac{1}{\lambda_D} - \frac{1}{2} \right). \quad (1)$$

Varying the relaxation parameter λ_D we have also studied diffusive transport for a set of bulk diffusivities ranging from $D_m=8.8 \times 10^{-4}$ to $D_m=1.5$.

In all simulations for both boundary rules, the obtained depth-averaged color concentration displays a Gaussian distribution, and the mean square displacement grows linearly in time. However, the vertical dependence of the concentration, as well as the diffusivity values, strongly depends on the BC used. While the concentration remains vertically homogeneous using BF, in Fig. 2 we show that using BB yields the undesired effect of a transient vertical variation of color. Two different situations can be distinguished in Fig. 2, namely, close to the mean position of tracer particles $\langle x \rangle$ or far from it. (Note that $\langle x \rangle$ is constant in time.) At $\langle x \rangle$ [Fig. 2(a)], the initial concentration gradient drives the tracer particles. Due to the bounce-back rule, particles close to the surface remain there longer, and the relative tracer concentration builds up. Shortly after, particles close to the surface diffuse toward the center of the channel, and eventually the concentration gradient in the vertical direction is smoothed out. On the other hand, far from the mean position of tracer

particles the situation is inverted. Bounce back at solid surfaces makes the tracer particles mostly arrive from the center of the channel, and a vertical concentration gradient develops. Thus, after several time steps, particles diffuse from the center toward the solid surfaces. At large times, the vertical gradient vanishes and the concentration becomes homogeneous across the channel.

Using BB, the diffusion coefficient strongly depends on the vertical size of the channel. Diffusive transport close to the solid surfaces is reduced due to the BB rule, yielding a smaller diffusion coefficient compared to bulk diffusivity. This effect becomes negligible when the gap is large enough or when the diffusivity is sufficiently small. In Fig. 3 we show the dependence of the diffusion coefficient (relative to D_m) on the size of the gap and bulk diffusivity. We also show that simulations using BF give $D=D_m$ for any size and D_m .

As mentioned, the undesired effects due to BB boundary conditions become less significant at small diffusivities. When using $D_m=8.8 \times 10^{-4}$ the deviation of the numerical value from the expected one is within 1%. However, the use of small diffusion coefficients allows large concentration gradients, which may result in numerical instability. Discrepancies between theory and simulations have been reported, in the LB model of miscible fluids, for values of D_m below 10^{-4} [20]. Also, for values of D_m below 10^{-4} , oscillations between negative and positive values of concentration have been observed [23]. Therefore, the region of parameter space where the model is fairly independent of the particular choice of the boundary condition rule is very close to being numerically unstable.

B. Taylor dispersion

Finally, we compute the asymptotic hydrodynamic dispersion when a mean flow is set within the channel. In this case, dispersion has two different contributions, one due to mo-

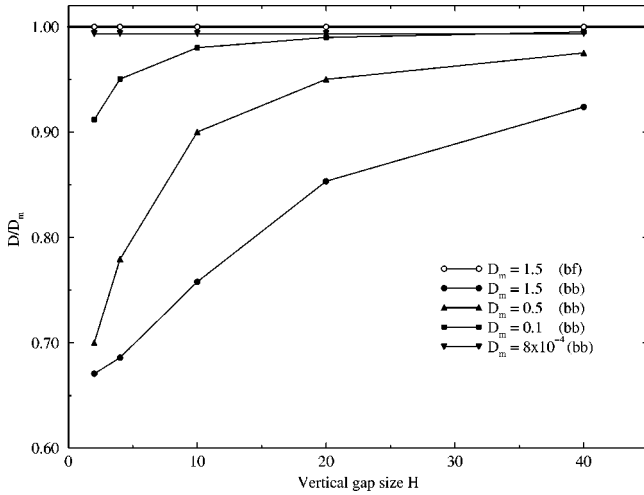


FIG. 3. Normalized diffusion coefficient D/D_m as a function of the vertical gap size. Solid symbols correspond to simulations using BB (for different bulk diffusivities). Open circles correspond to simulations using BF and $\lambda_D=0.2$. Results were obtained in a straight channel of length $L=512$. The initial condition is a Gaussian color distribution centered at $x=256$ and a width $\sigma^2=4.0$.

lecular diffusion and the other due to spatial variations of the fluid velocity, namely, Taylor dispersion [1]. Asymptotic analysis of Taylor dispersion in a two-dimensional channel of constant width H and mean flow velocity U gives the exact formula for the longitudinal dispersion coefficient [6],

$$D_{\parallel} = D_m + \frac{1}{210} \frac{U^2 H^2}{D_m}. \quad (2)$$

Introducing the Péclet number, which accounts for the relative magnitude of the convective and diffusive transport, $Pe = UH/D_m$, the previous equation can be rewritten as

$$D_{\parallel} = D_m \left(1 + \frac{Pe^2}{210} \right). \quad (3)$$

Concerning the numerical simulations, whether the BF rule is implemented or not, the Taylor regime for the longitudinal dispersion is expected to hold. However, the effective diffusivity is slowed down when a BB collision at solid surfaces is used. Thus, as the diffusivity is smaller, the characteristic homogenization time in the transverse direction becomes larger. In other words, we may expect Eq. (2) to hold, but where D_m is replaced by the effective diffusion coefficient in the channel D , as measured in diffusion simulations using BB rule (Sec. III A). In Fig. 4 we compare the numerical results with Eq. (2). There is very good agreement between the numerical results and the Taylor theory in both cases, using BB and BF as boundary rules. Let us remark that solid and dashed lines corresponds exactly to Eq. (2) with no adjustable parameter, and the only difference between them is the molecular diffusivity value. These results confirm the previous one, showing that the BB rule diminishes the diffusive transport and consequently enlarges the longitudinal hydrodynamic dispersion. A departure from Eq. (2) at large Péclet numbers can also be observed, where the

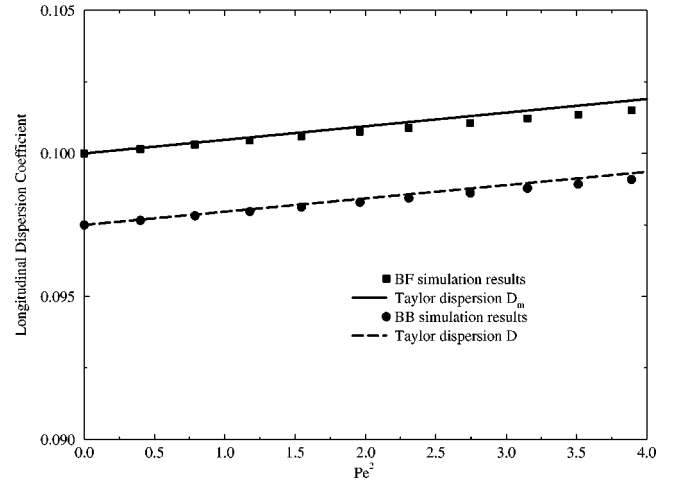


FIG. 4. Longitudinal dispersion coefficient as a function of the Péclet number squared. Solid line corresponds to Eq. (2). Dashed line also corresponds to Eq. (2) but using D measured in diffusion simulations (instead of D_m). Solid squares and circles refer to the numerical results using BF and BB, respectively. The channel grid is 16×1024 and the diffusion coefficient in bulk is $D_m=0.1$.

largest discrepancy is 0.3%. Similar results showing slightly smaller numerical values than theoretical ones have been previously reported [26].

As a conclusion to this section we may say that the effect of using the same BC on fluid and color distributions slows down the diffusive transport. This effect becomes appreciable when the system is narrow enough or the diffusion coefficient is large.

IV. SELF-AFFINE NARROW FRACTURES

We briefly review here the mathematical characterization of self-affinity. A more detailed discussion can be found in our previous work [27]. We consider a rock surface without overhangs, whose height is given by a single-valued function $z(x, y)$, where the coordinates x and y lie in the mean plane of the fracture. Self-affine surfaces [28] display scale invariance with different dilation ratios along different spatial directions (in contrast to self-similar surfaces which stretch the coordinates with equal ratios). Experiment indicates that isotropy can be assumed in the mean plane, implying that there is only one nontrivial exponent relating the dilation ratio in the mean plane to the scaling in the perpendicular direction, i.e.,

$$z(x, y) = \lambda^{-\zeta} z(\lambda x, \lambda y), \quad (4)$$

where ζ is the roughness or Hurst exponent [29]. In all cases the roughness exponent is chosen as the experimentally observed value $\zeta=0.8$.

We shall emphasize the limiting situation of narrow fractures, in which the two surfaces are very close to each other. Consider the situation in which a rock of lateral size L is fractured and the two surfaces are simply displaced by a distance $H \ll L$, perpendicular to the mean fracture plane, with no relative shift. The fluctuations (the difference be-

tween the maximum and minimum values of z) scale as $R \sim L^\zeta$. If H is the width of the fracture, then the limiting situation corresponds to $R \gg H$.

In narrow fractures, the correlation between the two sides is an important feature for the dispersion process, and we consider two possibilities. We first study fractures where the upper surface has been simply translated a distance H normal to the mean plane, so that the local aperture $a(x,y)$ equals the constant H . Alternatively, the two surfaces may have a relative lateral displacement d in the mean fracture plane, accompanied by a displacement H in the perpendicular direction, so that the two surfaces do not overlap. In this case the local aperture is given by the random variable

$$a_d(x,y) = z(x+d,y) - z(x,y) + h. \quad (5)$$

It turns out [30] that d is the lateral correlation length for fluctuations in the aperture, in the sense that $a_d(x,y)$ and $a_d(x+\Delta x,y)$ decorrelate for $\Delta x \gg d$.

Using the self-affine scaling law for the correlation function,

$$\sigma_z^2(\Delta x) = \langle [z(x,y) - z(x+\Delta x,y)]^2 \rangle = \phi(l) \left(\frac{\Delta x}{l} \right)^{2\zeta}, \quad (6)$$

where l is a microscopic length, say, a grain size, such that

$$\sigma_z^2(l) = \phi(l) \sim l^2, \quad (7)$$

we can estimate

$$\Delta Z(\Delta x) \equiv z(x,y) - z(x+\Delta x,y) \sim l \left(\frac{\Delta x}{l} \right)^\zeta. \quad (8)$$

For length scales $\Delta x \ll l$ it can be seen from the previous relation that $\Delta Z \gg \Delta x$ (given that ζ is smaller than 1). On the other hand, for length scales $\Delta x \gg l$, it is clear that $\Delta Z \ll \Delta x$. We consider l as the lower cutoff of the self-affine behavior in a real fractured system. This fact largely determines the convective-diffusive behavior, as we will discuss later.

In this paper we restrict ourselves to the two-dimensional case where the surface is invariant in the y direction, $z(x,y) = z(x)$, and the mean flow, when present, is forced in the x direction by a constant pressure drop. In a subsequent paper we will extend these calculations to fully three-dimensional fractures, but it is convenient, both conceptually and in numerical simulations, to regard the system as having a translationally invariant third dimension.

We use statistically self-affine surfaces with periodic boundary conditions. The periodicity is not a physically essential ingredient here, but has some calculational advantages in alleviating finite-size effects. The surface is generated by a Fourier synthesis method, based on power-law filtering of arrays of independent random numbers [27,31].

V. DIFFUSION IN NARROW FRACTURES

In this section we study diffusion in two-dimensional self-affine fractures. The approach will be based on the tortuosity

concept [32]. It is a common characteristic in fluid transport in porous media, and in fractures in particular, that the actual path followed by the fluid is very tortuous. In our fractured two-dimensional systems, a purely geometrical definition of tortuosity can be given, by considering the ratio of the shortest continuous paths between any two points within the fracture to the length of the system projected on to the main plane [33]. It is clear that, for narrow fractures, this ratio will approach the ratio between the length of the surface profile in the xz plane to the distance Δx between the two points. Then, if l_e is the true length between the two points separated a distance Δx , we can write, for the tortuosity,

$$T = \frac{l_e}{\Delta x}. \quad (9)$$

The tortuosity factor T accounts for the reduction in diffusivity, due to irregular geometries,

$$D = \frac{\Delta x^2}{2t} = \left(\frac{\Delta x}{l_e} \right)^2 \frac{l_e^2}{2t} = \frac{D_m}{T^2}, \quad (10)$$

where D_m is the free bulk molecular diffusion coefficient.

For the previous equation to be meaningful one should have a constant value of T , that is, independent of Δx . This is the case when the effective length l_e depends linearly on the size of the system, Δx . For self-similar surfaces, the relation between l_e and Δx defines the fractal dimension D_f , $l_e \propto \Delta x^{D_f}$. On the other hand, it has been shown that, for self-affine surfaces, there are several distinct definitions of fractal dimension [34–36]. However, for length scales well above l all fractal dimensions become $D_f = 1$ [34–36], and l_e is proportional to Δx . In this work we consider l as the lower cutoff of the self-affine behavior, and therefore, we only observe the situation where the tortuosity factor is constant. For the numerically generated self-affine surfaces used in this work, we tested the dependence of the effective length l_e on Δx . Using the method of ‘‘dividers’’ [29] to measure l_e , we obtain, in all cases, a linear relation between the dividers opening ϵ and $l_e(\epsilon)$, i.e., $D_B = 1$.

The fact that T is constant has some important consequences on diffusive transport. First, the relation between mean square displacement and time should be linear (after perhaps a transient time). Second, the distribution of tracer concentration should be asymptotically Gaussian and independent of the initial distribution of tracer. Finally, the correction due to tortuosity is strictly geometrical and therefore it should be independent on the actual value of the free bulk molecular diffusivity D_m .

In Fig. 5 we show the linear dependence of the mean square displacement on time for different values of the diffusion coefficient. Many other simulations with different values of D_m and H were performed, and in all cases a linear relation was obtained. In Fig. 6 we show how the same Gaussian distribution is approached at long times, starting from three different initial distribution of tracer particles. Finally, in Fig. 7 we show that the tortuosity factor is a strictly geometrical property, being clearly independent of the diffusivity of the tracer particles.

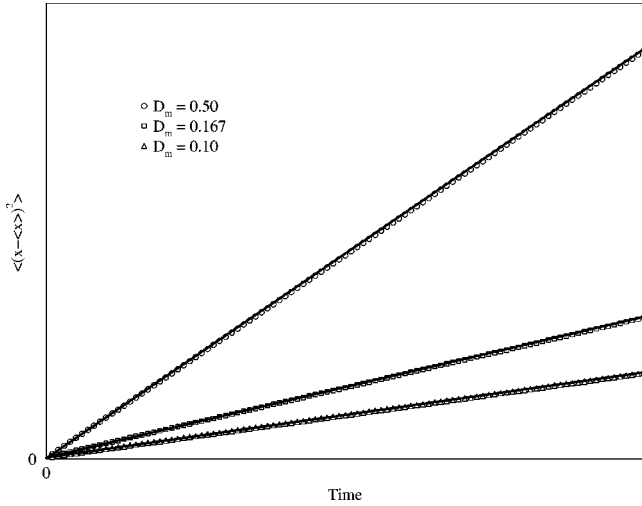


FIG. 5. Mean square displacement as a function of time for different diffusion coefficients. Simulations were performed in a system of length $L=512$ and separation between surfaces $H=4$.

Tortuosity dependence on the fracture width

In the previous section, we showed that the effect of surface roughness on diffusion can be accounted for by a purely geometrical property of the system, the tortuosity T . However, it remains to analyze the dependence of T on geometrical parameters that describe the system. Of particular importance is the dependence of T on the width of the fracture H .

The theoretical analysis presented here will closely follow the kind of approximation used in [27], where the fracture is divided into a sequence of quasilinear segments at varying orientation angles. First, we estimate a typical size ξ_{\parallel} in the direction of the mean flow over which the fluctuations in the vertical direction are small compared to the effective aper-

ture of the channel. A segment of length ξ_{\parallel} is roughly straight when $\Delta Z(\xi_{\parallel}) \sim l(\xi_{\parallel}/l)^{\zeta}$ is a small fraction of H , which yields

$$\xi_{\parallel} \sim l \left(\frac{H}{l} \right)^{1/\zeta}. \tag{11}$$

Returning to the entire fracture, each ξ_{\parallel} channel is oriented at some angle θ_i with respect to the mean plane and has effective aperture $a_i = H \cos \theta_i$ and length $\xi_{\parallel}^i = \xi_{\parallel} / \cos \theta_i$. Thus, we write, for the total length of the channel,

$$L_e = \sum_{i=1}^N \xi_{\parallel}^i = \xi_{\parallel} \sum_{i=1}^N \cos^{-1}(\theta_i). \tag{12}$$

Finally, taking into account that $N = L/\xi_{\parallel} \gg 1$ is the number of channels, we can convert the sum into an average over the distribution of angles, and write, for the tortuosity,

$$T = \frac{L_e}{L} = \langle \cos^{-1}(\theta) \rangle = \left\langle \frac{\sqrt{\xi_{\parallel}^2 + \Delta Z^2(\xi_{\parallel})}}{\xi_{\parallel}} \right\rangle \approx 1 + \frac{1}{2} \left(\frac{\sigma_z(\xi_{\parallel})}{\xi_{\parallel}} \right)^2, \tag{13}$$

where $\sigma_z^2(\xi_{\parallel}) = \langle \Delta Z^2(\xi_{\parallel}) \rangle$ [see Eqs. (6) and (8)] and, in order to estimate the cosine, we have used the fact that the channels present small vertical fluctuations.

A more precise evaluation can be obtained based on a Gaussian distribution of heights [27], as supported by experimental measurements [30] and, in fact, the actual distribution given by our numerical procedure for generating self-affine surfaces. In this case, the angular average is given by

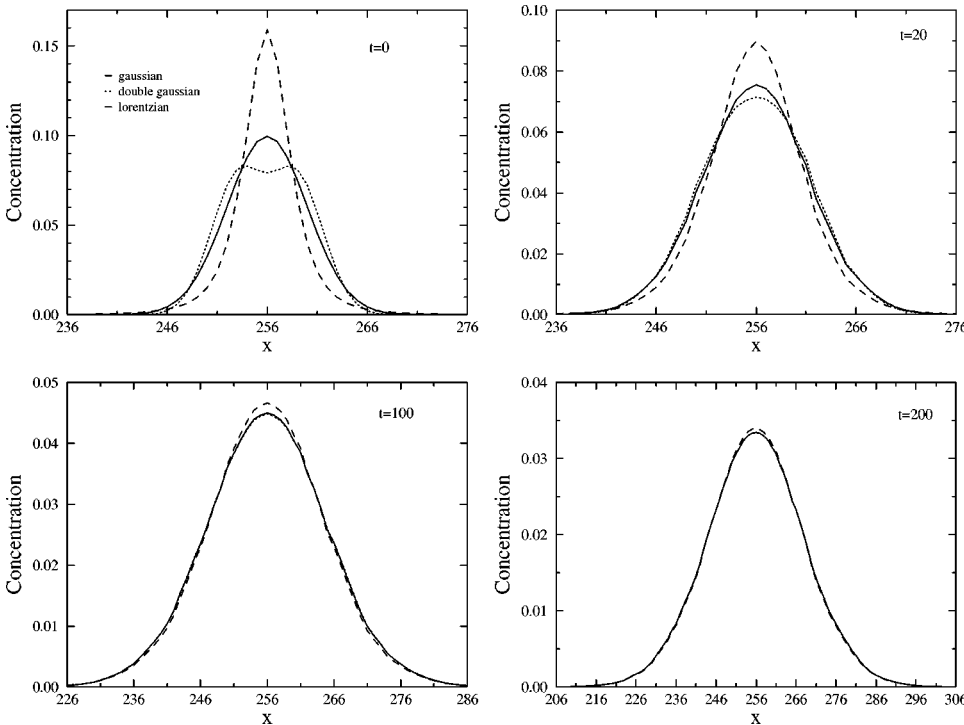


FIG. 6. Evolution of tracer concentration for different initial conditions: a Gaussian distribution, two Gaussians centered at $x_0 = 256 \pm 3$, and a Lorentzian distribution squared. The initial dispersion is in all cases $\sigma_0 = 4.0$ and $D_m = 0.5$.

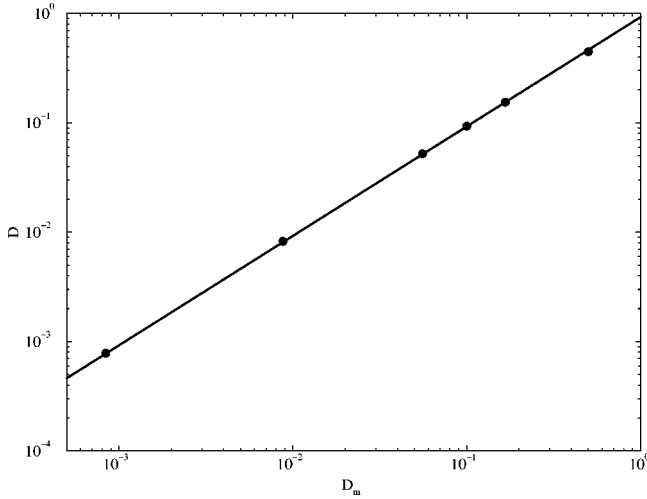


FIG. 7. Diffusion coefficient in the fractures D as a function of the free bulk diffusion coefficient D_m . The system length and width are $L = 512$ and $H = 16$. Solid circles correspond to simulations with $D_m = 5.0 \times 10^{-1}$, 1.67×10^{-2} , 1.0×10^{-1} , 8.77×10^{-3} , and 8.38×10^{-4} . The solid line corresponds to Eq. (10) with a tortuosity $T^2 = 0.93$.

$$\langle \cos^{-1} \theta \rangle = \int p(\Delta Z) \sqrt{1 + \left(\frac{\Delta Z}{\xi_{\parallel}} \right)^2} = x^{1/2} U\left(\frac{1}{2}; 2; x\right) \quad (14)$$

where $x = [\xi_{\parallel}^2 / 2\sigma_z^2(\xi_{\parallel})]$, and $U(a; b; x)$ is the *confluent hypergeometric function of the second kind* [37,38]. Therefore, we can get a more convincing evaluation of the tortuosity of a narrow two-dimensional self-affine fracture using the leading terms in the asymptotic representation of U for large x and Eq. (11) for the value of ξ_{\parallel} ,

$$T = \left[1 + \left(\frac{\phi(l)}{l^2} \right) \left(\frac{H}{l} \right)^{(2\zeta-2)/\zeta} \right]. \quad (15)$$

To compare the previous relation with the numerical results, let us first recast it in terms of the diffusion coefficient,

$$\frac{D_m - D}{D_m} \approx 2C_1 \left(\frac{H}{l} \right)^{(2\zeta-2)/\zeta}, \quad (16)$$

where we have added an adjustable parameter C_1 , which is expected to be of order 1.

In Fig. 8 we present the decrease in the diffusivity due to the tortuosity of the channel as a function of the distance between the opposite surfaces H . We find good agreement for the predicted exponent $(2\zeta - 2)/\zeta = -1/2$ (the roughness exponent is $\zeta = 0.8$). The only adjustable parameter is the coefficient C_1 , which is found to be $C_1 \approx 0.9$, in good agreement with the expected value.

In Fig. 9 we present the numerical results obtained for surfaces with smaller amplitude of the roughness (smaller value of l). In this case it is clear that the exponent differs from the predicted value. We believe that this discrepancy comes from the discretization of the surface in the numerical simulations. This discrete nature of the numerical surfaces

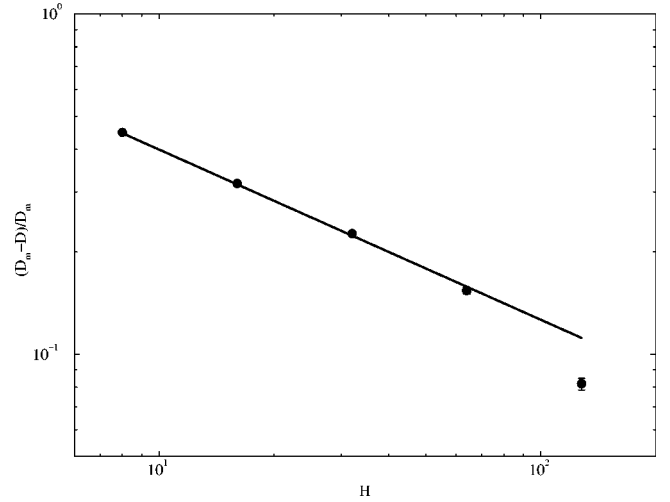


FIG. 8. Correction to the diffusivity due to tortuosity of the fractures as a function of the gap H . The solid line corresponds to Eq. (16) with $C_1 = 0.9$. The simulation parameters are $L = 512$, $\lambda_D = 0.5$, and $\zeta = 0.8$.

introduces a discrepancy with the continuous approach, which is more important for small vertical fluctuations in the surface height. However, we also show in Fig. 9 the theoretical correction to diffusive transport, computing the tortuosity factor directly through the numerically generated surfaces instead of using the asymptotic analysis. In this case good agreement is recovered and the only adjustable parameter $C_1 \approx 2$ is again of order 1 (and in agreement with previous results [27]). Similar results were obtained using several intermediate values for the surface fluctuations in height, where the reduction in diffusivity is always in agreement with the correction due to the tortuosity of the channels. In addition, we found that the decrease in diffusivity is, in all

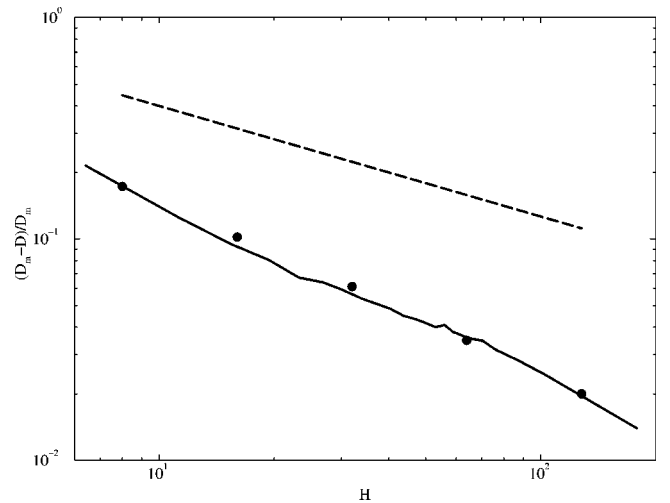


FIG. 9. Correction to the diffusive transport when the surface fluctuations are small. The solid line is the correction due to the tortuosity of the channel, measured from the numerically generated surfaces. The dashed line corresponds to the observed reduction in diffusivity when the fluctuations are larger and the dependence is correctly reproduced by Eq. (16).

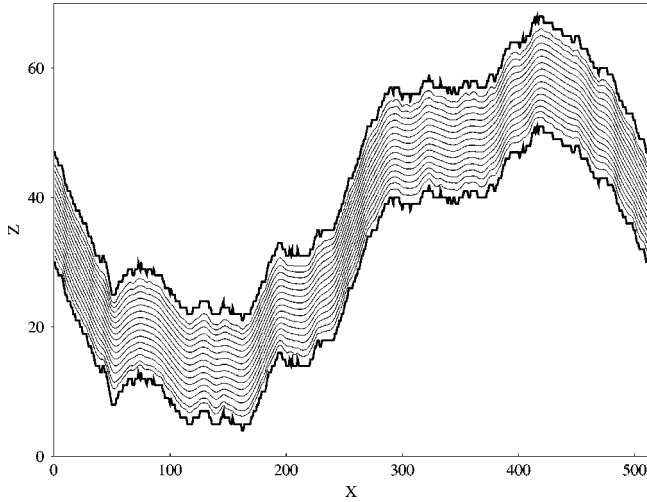


FIG. 10. Streamlines inside a fracture of width $H=16$, length $L=512$, and no lateral shift between complementary surfaces. Note that the closer the angle of the surface to $\pi/2$, the narrower the effective width becomes.

cases, well described by a power law (where the power-law exponent decreases slightly with the amplitude of the surface fluctuations), for which we have no explanation.

VI. DISPERSION IN NARROW FRACTURES

In this section we address the case of Taylor hydrodynamic dispersion in narrow fractures. First, we will analyze the case where the two sides of the fracture are displaced normally to the mean fracture plane, and then we will turn to the case where there is a lateral shift as well.

When the two complementary surfaces are simply displaced vertically by a distance $H \ll L$, the vertical aperture of the system is constant everywhere. Nevertheless, the flow field differs from one in a straight channel, due to variations in the local width of the channel normal to the mean flow direction. In Fig. 10 we show a set of streamlines inside a fracture, where the effect of the varying effective aperture of the fracture is evident (aperture normal to the mean flow). Moreover, in [27] we show that the complex geometry of the fracture gives rise to low-velocity zones (close to depressions and corners), reducing the permeability of the system. In order to describe the dispersion process we need to obtain a measure of the fraction of the system that is subject to convection. To this end we will make use of the Λ parameter [39,40], which is directly related to transport and measures the *dynamically connected* part of the pore space in porous media [41,42]. Following Ref. [42], we write Λ in terms of the permeability and tortuosity of the system,

$$k = \frac{\Lambda^2}{12T^2}. \quad (17)$$

Note that defining a characteristic length as the ratio between pore volume V and surface area S would yield $V/S = H/T \neq \Lambda$, which does not depend on the effects exerted on the fluid flow by the complex geometry of the fracture.

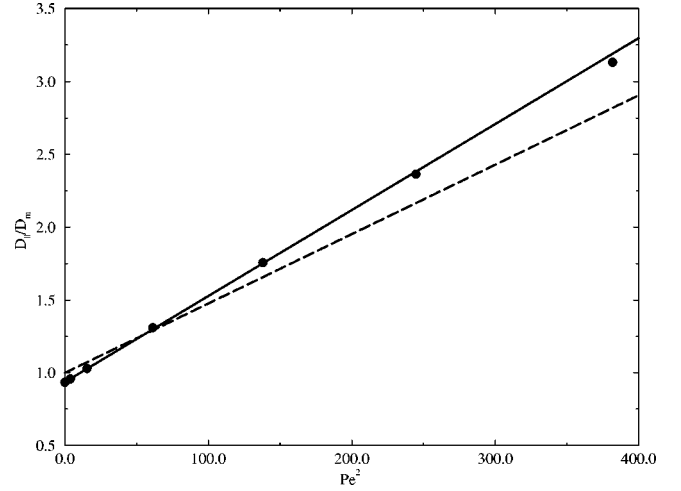


FIG. 11. Dispersion coefficient as a function of the Péclet number squared. Solid line corresponds to the best fit using Eq. (18), with D_m and Λ as adjustable parameters. Dashed line corresponds to Taylor dispersion in a straight channel with equal aperture $H=16$.

Now, assuming that we have a winding channel of length L_e , effective aperture for convective transport Λ , and actual aperture $A = H/T$ (given by volume conservation), we may apply the same reasoning as in Sec. III B to get the dispersion coefficient. After replacing H by the width of the effective channel H/T , U by the mean velocity in the convective part of the channel UH/Λ , and taking into account the tortuosity, we obtain

$$D_{\parallel} = \frac{D_m}{T^2} \left[1 + \frac{\text{Pe}^2}{210} \left(\frac{H}{\Lambda T} \right)^2 \right]. \quad (18)$$

Thus, to see how well the Λ parameter can be used to estimate the dispersion, we will compare the values obtained both from dispersion measurements [Eq. (18)] and from the permeability [Eq. (17)].

In Fig. 11 we show the numerical results obtained for the dispersion coefficient when varying the injection rate. The linear behavior shows that, as expected, Taylor dispersion is governing tracer spreading. The fracture gap is $H=16$, the length of the system is $L=512$, and the relaxation parameter used is $\lambda_D=1.9$. The molecular diffusivity and the lambda parameters obtained from the best fit are $D_m = (8.86 \pm 0.01) \times 10^{-3}$ which differs by only 1% from the theoretical value, and $\Lambda = 13.4 \pm 0.1$. On the other hand, from the flow rate computed in numerical simulations and estimating the permeability by Eq. (17), we get $\Lambda = 15.3 \pm 0.2$.

We now turn to shifted surfaces. In the presence of a small lateral shift d between complimentary surfaces, most of the previous discussion remains valid. The local aperture now varies with position and H is the average aperture of the channel. The difference in height between surfaces at any point x along the channel is of order d^ξ , while the vertical excursion of the fracture between points separated a distance Δx is $(\Delta x)^\xi$. Therefore, at large length scales $\Delta x \gg d$, the fracture may be considered as a winding channel of length L_e and effective aperture Λ and where the ratio between the

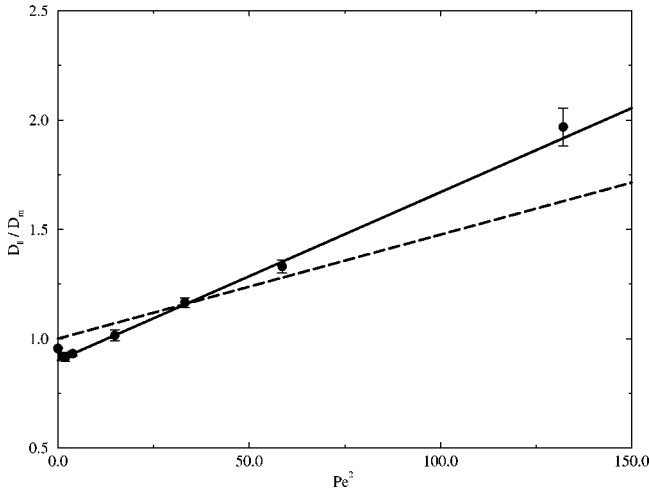


FIG. 12. Dispersion coefficient as a function of the Péclet number squared. Solid line corresponds to the best fit using Eq. (18), with D_m and Λ as adjustable parameters. Dashed line corresponds to Taylor dispersion in a straight channel with equal aperture $H = 16$.

length of the channel L_e and the system length L is the tortuosity factor.

In Fig. 12 we show the dispersion coefficient, as a function of the Péclet number. The two fracture surfaces are vertically displaced by $H=16$ and laterally shifted by $d=8$. As expected, we observed a linear dependence, in agreement with Taylor-like spreading. From the best fit of the numerical results we obtain $D_m = (8.5 \pm 0.1) \times 10^{-3}$, which differs less than 3% from the theoretical one ($\lambda_D = 1.9$), and $\Lambda = 14.6 \pm 0.2$, whereas by means of flow rate data computed in numerical simulations and Eq. (17) for the permeability, we obtain $\Lambda = 11.7 \pm 0.5$.

Even though estimated values of Λ are in fairly good agreement (within a 20% discrepancy), it is also clear that the Λ parameter fails to completely predict the enhancement of dispersion due to the complex geometry of the fractures. Nevertheless, we believe that the presence of low-velocity zones is the only possible feature that accounts for the enhancement in the spreading of tracer particles.

Let us note that the uncertainty in the computed dispersion coefficient is considerably larger than in the case where there is no lateral shift. It has been shown, in three-dimensional fractures and under a lubrication approximation for the velocity field, that a lateral shift yields geometric dispersion for tracer particles advected along the flow [43]. This effect is due to a different mean velocity along different streamlines. In our case, the two-dimensional nature of the fractures prevents the presence of geometric dispersion, given that the height-averaged velocity is constant throughout the system. However, an analogous effect appears when averaging over different fractures, giving rise to a large dispersion in the computed mean velocity and dispersion coefficient. In fact, from the previous discussion an uncertainty proportional to the mean velocity is expected when averaging the dispersion coefficient (corresponding to a geometric dispersion term in fully three-dimensional fractures).

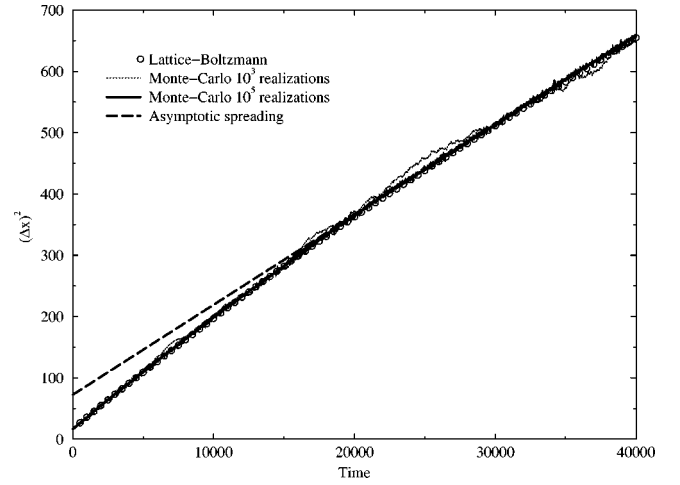


FIG. 13. Mean square displacement of tracer particles as a function of time, in a single fracture (mean aperture $H=16$, shift between surfaces $d=8$, length $L=512$, mean velocity $U \approx 10^{-3}$, $D_m = 0.008771$). Solid line and open circles correspond to numerical MC and LB simulations, respectively. Dashed line is the best linear fit for large times, i.e., the asymptotic linear spreading of the tracer ($D = 7.4 \times 10^{-3}$).

In order to validate the dispersion results obtained by means of the LB method, we shall now compare them with results computed via a Monte Carlo (MC) approach to the dispersion process. In the MC method, one follows the displacement of a large number of particles, or random walkers, moving in a two-dimensional fracture. The motion of each particle is a combination of the effects of molecular diffusion and convection (we assume, as in LB simulations, that tracer particles move independently of each other). In time Δt , a particle is displaced according to

$$\Delta \mathbf{x} = \mathbf{u}(\mathbf{x}) \Delta t + \hat{\mathbf{n}} (4D_m \Delta t)^{1/2}, \quad (19)$$

where $\mathbf{u}(\mathbf{x})$ is the velocity field obtained by the LB method, $\hat{\mathbf{n}}$ is a unit vector with random orientation, and the amplitude of the random steps has been chosen so that the variance of any coordinate is $2D_m \Delta t$ [44–46]. Boundary conditions at solid surfaces are implemented as in [44], where those random steps that would take the particle outside the channel are suppressed. The sequence of steps is repeated while recording the distance Δx from the initial position of the particle. The process is repeated for a large number of particles and average values are computed.

We found excellent agreement between the two methods. In Fig. 13 we compare the mean square displacement as a function of time obtained using LB and MC methods. The agreement is evident, and it can be seen that after releasing 10^5 particles in the MC simulations, the noise is negligible. Both simulations correspond to a fracture of mean aperture $H=16$, length $L=512$, and a lateral shift between surfaces $d=8$. It is also interesting to note, in Fig. 13, a change in the slope at time $t \sim 20000$, which approximately corresponds to the characteristic time for transverse diffusion across the aperture $\tau_D \approx H^2/2D_m \sim 15000$. Therefore, this marked change in slope is showing the transition towards Taylor-like spreading at times larger than τ_D .

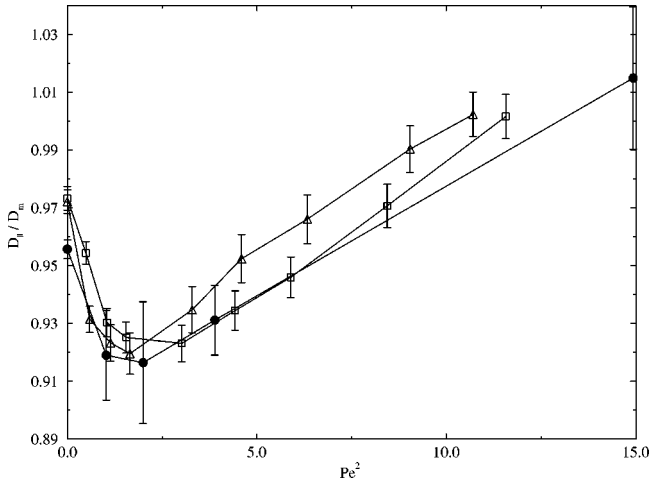


FIG. 14. Dispersion coefficient at low Péclet numbers. Different results correspond to different simulation methods. Solid circles correspond to LB method. Squares correspond to MC simulations where the velocity was computed using LB. Triangles correspond to MC simulations using the velocity field given by the lubrication approximation.

Dispersion at small Péclet numbers

In a straight channel, the presence of convection increases the dispersion of tracer particles. The same effect is usually found in porous media, including fracture systems. However, in the case where surfaces are laterally shifted and at very small Péclet number, we observed the opposite behavior. That is, the presence of convective transport inside the fractures reduces the dispersion of tracer particles. This effect can be observed in Fig. 12; at very small Pe the dispersion coefficient grows as the flow rate decreases. In order to validate this observation we simulate the dispersion process with two other methods. The first one is the MC method presented before. The second method is a variation of the MC where, instead of using the velocity field computed by means of LB simulations, we use lubrication approximation for velocities. In the lubrication approximation the velocity $u(x,z)$ is given by

$$u(x,z) = \frac{6Q}{H^3(x)} z[H(x) - z], \quad (20)$$

where $H(x)$ is the local aperture of the fracture.

In Fig. 14 we show the results obtained using the three different methods in a range of Pe from 0 to 4. The agreement between methods is excellent and all show an initial decrease in dispersion due to the presence of weak convective transport. We believe that, at very low velocities, the main effect of convective transport is to carry out tracer from *low-velocity* zones, thus reducing dispersion. This explanation is supported by the fact that the lubrication approximation yields very similar results. (Note that this approximation assumes a local Poiseuille profile without accounting for possible stagnant zones.) Unfortunately, the small Péclet numbers at which this surprising effect arises make it very difficult to be experimentally measured.

VII. CONCLUSIONS

In the first place, we have presented a set of boundary conditions to describe diffusive transport within the lattice-Boltzmann method. We tested this boundary rule in two situations, simple diffusion and Taylor dispersion in two-dimensional straight channels. We showed that the proposed bounce-forward rule improves the accuracy of the method and does not possess the undesirable effects of the bounce-back rule, i.e., dependence of the diffusion coefficient on the aspect ratio of a straight channel and transient concentration gradients near solid walls. Even though the accuracy might be recovered in the BB case using small diffusivities, we showed that this option leads the simulations towards the numerical instability border.

We then turn to study diffusive transport in two-dimensional self-affine fractures. First, we showed that the slowdown in diffusive transport can be accounted for by the purely geometric tortuosity factor. Our numerical simulations have verified all the implications of this result, that is, linear spreading in time, Gaussian distribution of tracer, and independence of geometrical effects on the actual value of the diffusivity. Second, using analytic arguments in the limit of small aperture fluctuations, we have obtained an expression for the tortuosity in terms of the fracture gap and the Hurst exponent characterizing the fracture surface. Numerical simulations verify the validity of the theoretical approach even when the discrete nature of the surface seems to affect the asymptotic scaling law.

Finally we studied tracer dispersion in fractures in the presence or not of a lateral shift between complementary surfaces. In both cases we showed that tracer spreading can be described as analogous to Taylor-like dispersion in a straight channel. In the case without a lateral shift we showed that the enhancement in dispersion can be mostly understood assuming an effectively reduced aperture for fluid transport due to the rugosity of the surface. The Λ parameter measuring this effective aperture, and computed from permeability measurements, was shown to be similar to that estimated from dispersion measurements. We also presented a result showing a decrease in tracer dispersion when convective transport is set in the fracture. This last observation was obtained in the framework of three different numerical approaches.

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