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Particle-tracking simulations of anomalous transport in hierarchically fractured rocks

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ABSTRACT

Complex topology of fracture networks and interactions between transport processes in a fracture and the ambient un-fractured rock (matrix) combine to render modeling solute transport in fractured media a challenge. Classical approaches rely on both strong assumptions of either limited or full diffusion of solutes in the matrix and simplified fracture configurations. We analyze fracture-matrix transport in two-dimensional Sierpinski lattice structures, which display a wide range of matrix block sizes. The analysis is conducted in several transport regimes that are limited by either diffusion or block sizes. Our simulation results can be used to validate the simplifying assumptions that underpin classical analytical solutions and to benchmark other numerical methods. They also demonstrate that both hydraulic and structural properties of fractured rocks control the residence time distribution.

1. Introduction

Solute transport in fractured porous media often exhibits anomalous (non-Fickian) characteristics that, if ignored, can compromise both site characterization and model reliability (Berkowitz, 2002; Carrera et al., 1998; Neuman, 2005; Zhou et al., 2007). Spatial and/or statistical heterogeneity of fracture networks and interactions between transport processes in a fracture and the ambient un-fractured rock (matrix) are two mechanisms that are responsible for this non-Fickian behavior. The former affects hydraulic properties of fractured rocks (Bonnet et al., 2001; Bour and Davy, 1999; Davy et al., 2006, 2010; de Dreuzy et al., 2001; Doughty and Karasaki, 2002), while the latter controls long-term transport characteristics (Birgersson and Neretnieks, 1990; Dershowitz and Miller, 1995; Haggerty et al., 2000; Neretnieks, 1980). Solutes are delayed by exchange between the high-velocity fracture paths and the poorly permeable matrix as well as by solute adsorption within the matrix. Fracture-matrix exchange is driven by (1) solute dynamics within the fractures conditioning the transfer to the matrix blocks (Carrera et al., 1998; Hamm and Bidaux, 1996; Hassanzadeh and Pooladi-Darvish, 2006), (2) geometrical structures of the blocks (Crank, 1975; Dershowitz and Miller, 1995; Warren and Root, 1963) and (3) heterogeneity of transfer processes and porosity (Bai et al., 1993; Haggerty and Gorelick, 1995; Lagendijk et al., 2000).

While both the network structure and natural (or experimental) physical conditions affect fracture-matrix exchange and thus the residence time distribution, classical models generally focus on just one of these two mechanisms and ignore (or strongly simplify) the other. On the one hand, the dual-porosity approach assumes that fractures and ambient matrix can be independently homogenized and that exchange between them depends on a single coefficient (Barenblatt and Zheltov, 1960; Warren and Root, 1963). On the other hand, the single fracture approach reduces fracture networks to a single fracture or a set of parallel fractures embedded in a homogeneous matrix (Sudicky and Frind, 1982; Tang et al., 1981). These approaches employ simplified models of diffusion in matrix blocks, ignoring (or simplifying) the effects of block shapes and sizes, and fracture hydraulics. More recent modeling frameworks employ shape factors (Hassanzadeh et al., 2009; Lim and Aziz, 1995), multi-rate mass transfer (Haggerty and Gorelick, 1995) or memory functions (Carrera et al., 1998) to account for the fracture-matrix exchange in more realistic settings. Yet their reported applications are mostly limited to idealized systems, such as layered, cylindrical or spherical exchange. Roubinet et al. (2010) proposed a particle-tracking algorithm that is especially adapted to heterogeneous fractured porous media with multiple matrix block sizes.

We deploy the Roubinet et al. (2010) algorithm (code PERFORM) to simulate solute migration in fracture networks exhibiting an evolving range of matrix block distribution, in several transport regimes. Our analysis aims to (1) establish benchmark solutions of solute transport in complex fractured media characterized by a

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distribution of matrix bock sizes, (2) evaluate the validity of classical modeling concepts, and (3) identify characteristic diffusion regimes of solute transport in complex fractured media. Section 2 contains a formulation of benchmark problems, and the numerical algorithm for solving these problems is described in Section 3. The resulting breakthrough curves are presented in Section 4, and used in Section 5 to identify various diffusion regimes.

2. Formulation of benchmark problems

The Sierpinski lattices are hierarchical fractal structures that exhibit high degrees of connectivity imposed by a set of continuous elements (Doughty and Karasaki, 2002). Several studies have demonstrated that the high degree of connectivity of these structures provides an adequate representation of the heterogeneity of natural fractured media (Davy et al., 2006; de Dreuzy and Davy, 2007; Doughty and Karasaki, 2002; Sahimi, 1993). The Sierpinski lattices are generated by recursively shrinking and replicating a pattern through scales. Structures are controlled by a density parameter directly linked to the fractal dimension of the resulting structure (de Dreuzy and Davy, 2007) and the level of recursive divisions k. We are mostly interested in the extent of the block-scale distribution parameterized by k and consider three structures with $k=1$, 2, or 3 (Fig. 1).

The basis configuration ($k=1$) corresponds to a regular fracture network, which is used as a reference. Increasing the magnitude of k ($k=2$ and $k=3$) increases structure heterogeneity. In what follows, we refer to the three block geometries generated by the case $k=3$ in Fig. 1 as large, medium and small blocks.

Unless specified otherwise, simulations are conducted with the following parameters: the domain length is set to $L=100$ m, the fracture aperture to $2b=10^{-4}$ m, the matrix porosity to $\phi_m=0.1$, and the matrix diffusion coefficient to $D_m=10^{-8}$ m^2/s (corresponding to molecular diffusion coefficient multiplied by a tortuosity factor). Periodic boundary conditions and a uniform head gradient (∇h) are applied in the vertical and horizontal directions respectively. Simulations are conducted for several values of the head gradient corresponding to the fracture flow velocity $v=10^{-1}$ m/s (Fast Flows), 10^{-3} m/s (Medium Flows) and 10^{-4} m/s (Slow Flows) for the simplest configuration (Fig. 1, $k=1$). These velocities have been selected to identify characteristic regimes and their extension for the range of velocities typically used for field tracer tests, i.e., 10^{-2}–10^{-6} m/s (Zhou et al., 2007).

Solute transport is analyzed through the residence time distribution within the domain. Particles are injected at the inlet (left side of the domain) within the fractures and their residence time is recorded at the domain outlet. The residence-time distributions from 10.000 particles are similar to those obtained from 100.000 particles and are presented in Section 4.

3. Simulation algorithm

Classical solute transport models rely on simplified network structures and/or diffusion regimes. To simulate solute transport on a large range of structural and hydraulic properties, we use the particle-tracking approach of Roubinet et al. (2010) that is specifically designed for highly heterogeneous fractured porous media. This modeling method enables one to handle (1) heterogeneous hydraulic properties of fracture networks, (2) unlimited or limited diffusion within matrix blocks, and (3) a wide distribution of matrix block sizes.

For a particle advecting during the time t_a in the fracture, its diffusion time t_{diff} in the surrounding infinite matrix is estimated by (Painter and Cvetkovic, 2005)

$$t_{diff}=\left(\frac{\phi_m\sqrt{D_m}}{2\alpha b}t_a\right)^2 \tag{1}$$

where ϕ_m and D_m are the matrix porosity and diffusion coefficient respectively, b is the fracture half-aperture, and $\alpha=\mathrm{erfc}^{-1}(U[0,1])$ with $U[0,1]$ denoting a uniform random number in the interval [0,1]. The corresponding penetration depth x_{diff} into the matrix is

$$x_{diff}=\frac{\phi_m D_m}{\sqrt{2}\alpha b v}l \tag{2}$$

where l is the length of the fracture segment and v is the fracture flow velocity. We define a fracture segment as the segment delimited by two fracture intersection points.

The assumption of infinite matrix corresponds to a diffusive regime not limited by structural properties. Expressions (1) and (2) remain valid as long as particles do not reach one of the neighboring fractures by diffusion through the matrix blocks. This condition can be expressed as $x_{diff}<B$, where B is the distance from the initial fracture to the closest neighboring fractures. For the specific square matrix blocks configuration in Fig. 1, the closest neighboring fracture of a fracture segment of length l is located at the same distance $B=l$. Solute diffusion is thus not limited by structural properties for small values of the characteristic ratio β_1 expressed as

$$\beta_1=\frac{\phi_m D_m}{bv} \tag{3}$$

and corresponding to a modified inverted Péclet number where the characteristic length is the fracture aperture instead of the fracture length.

For larger values of the characteristic ratio β_1, diffusion may be limited by the size of the block, and particles may transfer to a neighboring fracture through the matrix block one (or several) time(s). The required characteristic diffusion time t_B to cross the

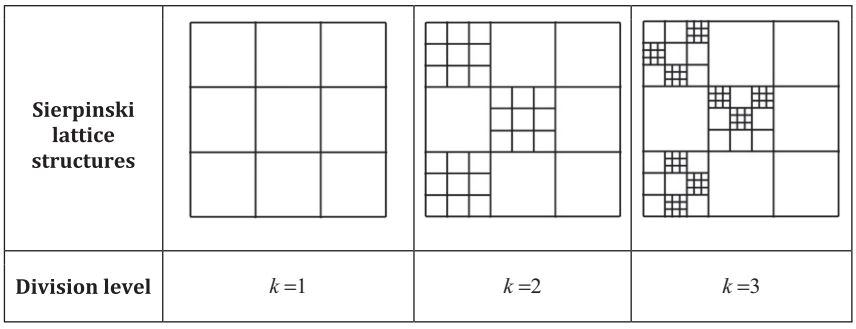

Fig. 1. The Sierpinski lattices with evolving ranges of the block size distribution for domain size $L=100$ m and fracture aperture $2b=10^{-4}$ m.