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Non-Fickian dispersion in a single fracture

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ABSTRACT

Solute transport in fractured rocks is of major interest in many applications, from the petroleum industry to ground water management. This work focuses on the dispersion process in a transparent replica of a real single fracture. The fracture exhibits strong changes in heterogeneity, with the first half very heterogeneous and the second half fairly homogeneous. Three models have been used to interpret the tracer experiments: the classical advection-dispersion equation (ADE), the continuous time random walk (CTRW), and the stratified model. The main goals were to test these models and to study possible correlations between fitting parameters and heterogeneities. As expected, the solution derived from the ADE equation appears to be unable to model long-time tailing behavior. On the other hand, the results confirm the CTRW robustness and the coefficient β seems well correlated to heterogeneities. Finally, the stratified model is also able to describe non-Fickian dispersion. The parameters defined by this model are correlated to the heterogeneities of the fracture.

1. Introduction

Solute transport in fractured rock is of great interest in groundwater pollution, CO_2 sequestration, and oil recovery. One of the main research areas in hydrogeology is the selection of repository sites, either for nuclear waste or CO_2 sequestration in geological formations. Integrity of reservoirs, which may present imperfections such as fractures and faults, is therefore a major issue, which makes flow characterization in fractures essential. Experiments on transparent replica of a real fracture have been wildly used to study two-phase flow (Persoff and Pruess, 1995), aperture fields (Detwiler et al., 1999, Isakov et al., 2001), and dispersion (Brown et al., 1998; Detwiler et al., 2000; Lee et al., 2003). Most of the later works focused on the outlet breakthrough curves, analyzing the dispersion from the overall fracture properties. The goal of this paper is the study of hydrodynamic dispersion due to aperture field heterogeneities through the interpretation of the breakthrough curves evolution along the flow direction. One-dimensional solutions were derived from three models: the advection-dispersion equation ADE, the continuous time random walk CTRW and the stratified model. Their ability to fit the breakthrough curves and the variation of their fitting parameters with the distance was studied. Although the experiment presented here is restrictive because of the uniqueness of the fracture, this work shows how model parameters may correlate with aperture field heterogeneity. The experiment was performed with non-reactive solute in a single-fracture with impermeable walls. The Peclet number was high enough to neglect molecular diffusion and to focus on the impact of the heterogeneities.

2. Theory

2.1. The advection-dispersion approach

The basic mass balance equation in one dimension is:

$$\frac{\partial C}{\partial t}+\frac{\partial F}{\partial x}=0 \tag{1}$$

where C is the average solute concentration and F is the mass flux per unit area. In a piston-like displacement without dispersion, the relationship between the flux and the concentration is simply $F = UC$, with U the average fluid velocity. In real tracer flow, the common approach for

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expressing the flux in accordance with the concentration is based on a Fickian law as follows (Bear, 1988; Dullien, 1992):

$$F = UC - D\frac{\partial C}{\partial x} \tag{2}$$

This leads to the well-known advection-dispersion equation, ADE (Bear, 1993):

$$\frac{\partial C}{\partial t} + U\frac{\partial C}{\partial x} = D\frac{\partial^2 C}{\partial x^2} \tag{3}$$

where D is the longitudinal hydrodynamic dispersion coefficient. With smooth walls and a constant aperture, D is the Taylor–Aris dispersion coefficient (Brenner and Edwards, 1993; Dutta and Leighton, 2001), $D_m + fU^2B^2 / D_m$, where D_m is the molecular diffusion coefficient, B is the aperture, and f is a constant that depends on the cross-sectional geometry. For a fracture with varying apertures, D has a similar form, $D_m + \alpha U$, where α is the dispersivity (Bear, 1993). For a homogeneous medium and for given initial and boundary conditions, analytical solutions for Eq. (3) may be easily derived. In the case of a step injection in a medium initially without solute:

$$\begin{cases} \text{if } t \le 0 \text{ then } C(x,t) = 0 \ \forall x \\ \text{if } t > 0 \text{ then } C(x,t) = C_0 \quad \text{for } x = 0 \end{cases} \tag{4}$$

the solution of Eq. (3) is the well-known Ogata–Banks solution (Ogata and Banks, 1961):

$$\frac{C}{C_0} = \frac{1}{2}\left(\mathrm{erfc}\left(\frac{x - Ut}{2\sqrt{Dt}}\right) + \exp\left(\frac{Ux}{D}\right)\mathrm{erfc}\left(\frac{x + Ut}{2\sqrt{Dt}}\right)\right) \tag{5}$$

This solution assumes a constant dispersion coefficient in time and space in the range [0,x], and therefore gives reasonable results for homogeneous media. Although very popular, the ADE is known to fail with heterogeneous media since the early 60's (e.g., Coats and Smith, 1964). In particular, it is unable to predict early breakthrough time and long-time tailing, referred to as non-Fickian behavior (for an overview see, e.g., Sahimi, 1993; Bodin et al., 2003).

2.2. The continuous time random walk approach

The continuous time random walk theory (CTRW) has been developed specifically to model conservative tracer transport where behavior is non-Fickian (Berkowitz and Scher, 1998; Berkowitz et al., 2001; Margolin and Berkowitz, 2004; Berkowitz et al., 2006). In one dimension, the particle dispersion over a distance x in time t is modeled by a transition probability density function $\psi(x,t)$, which is assumed to be stationary. Details of the theory and mathematical development may be found in the references cited above. Following Berkowitz et al. (2001), $\psi(x,t)$ may be approximated by a power law decay, $t^{-1-\beta}$, where β is a parameter that characterizes the dispersion regime. For $\beta>2$, the process is Fickian and the CTRW is equivalent to the classical advection-dispersion model. If $2>\beta>1$, the process is no longer Fickian; the location of the center of mass of the tracer front, x_0, travels at a constant velocity and the standard deviation scales as $t^{(3-\beta)/2}$. If $1>\beta>0$, the ratio of x_0 and the standard deviation is constant and both scale as t^{β}. For a step injection condition, there are analytical solutions that depend on the value of β (Berkowitz et al., 2001):

$$\frac{C}{C_0}(\xi\nu) = \frac{1}{\beta}\left(1 + \frac{1}{\pi}\sum(-\xi)^n\frac{\Gamma(n\nu)}{\Gamma(n+1)}\sin(\nu\pi n)\right)$$
$$\text{with} \begin{cases} \xi = \dfrac{(1-t/\tau)}{r} \quad \text{and } \nu = \dfrac{1}{\beta} \quad \forall \quad 2>\beta>1 \\ \xi = \left(\dfrac{t}{\tau} + r\right)^{-\beta} \quad \text{and } \nu = \beta \quad \forall \quad 1>\beta>0 \end{cases} \tag{6}$$

where β, τ, and r are three adjustable parameters. For a distance L_x, τ is the mean transition time, and r is related to the front spreading. If there are strong heterogeneities, the center of mass of the tracer front does not flow at the average fluid velocity, and τ is not necessarily the ratio between L_x and the average fluid velocity. According to Berkowitz et al. (2001), the mean velocity of the tracer front is mainly the average fluid velocity for $\beta>1$. This approximation improves as β increases above 1, but it is not usually verified for $\beta<1$. With a stationary density function, β, τ, and r may be determined at a distance L_x and derived at any other distance λL_x. The value β remains constant. τ scales as: $\lambda^{1/\beta}\tau$ for $\beta<1$ and $\lambda\tau$ for $\beta>1$. r scales as: $\lambda^{(1-1/\beta)}r$ for $\beta<1$ and $\lambda^{(1-\beta)}r$ for $\beta>1$.The C code implementation of solution (6) developed by Berkowitz (http://www.weizmann.ac.il/ESER/People/Brian/CTRW/) has been used to fit our data (Section 4).

2.3. The stratified medium approach

This approach is based on the idea of replacing a heterogeneous porous medium with an equivalent stratified medium (Fourar, 2006). The displacement of the tracer in each layer is assumed to be piston-like, with no dispersion, molecular diffusion, or mass transfer across layers. The key parameter characterizing tracer transport is shown to be the heterogeneity factor, defined as the ratio of the standard deviation to the mean permeability, also known as the variation coefficient.

We first consider a perfectly stratified medium with a uniform porosity. The permeability of the layers is randomly distributed, and the flow is parallel to the layers. Pore-scale dispersion and molecular diffusion are negligible. For a step injection at constant flow rate Q and concentration C_0 at $x=0$, the concentration at position x and time t is given by:

$$C(x,t) = C_0\int_{K(x)}^{K_{\max}} G(K)dK \tag{7}$$

where $G(K)$ is the probability distribution of the permeability, $K_{\max}$ is the maximum permeability value, and $K(x)$ is the layer's permeability where the tracer front reaches position x at time t. Taking a normal distribution defined for $K\in[0, \infty]$:

$$G(K) = \frac{1}{\sigma\sqrt{2\pi}}\exp\left(-\frac{(K - \langle K\rangle)^2}{2\sigma^2}\right) \tag{8}$$

and using the fact that:

$$K(x) = \frac{x\langle K\rangle}{Ut} \tag{9}$$

it follows that:

$$C(x,t) = \frac{C_0}{2}\mathrm{erfc}\left(\frac{x/Ut - 1}{H_f\sqrt{2}}\right) \tag{10}$$