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Technical note

Assumptions of the analytical solution for solute transport in a fracture–matrix system

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1. Introduction

In the past decades, a number of analytical solutions were developed to model solute or contaminant transport processes in a single fracture–matrix system.^{1–4} The first and widely applied analytical solution for solute transport in a simplified single fracture located in a semi-infinite porous rock matrix was put forward by Tang et al.,² considering mechanisms of advection, dispersion, matrix diffusion, sorption and decay processes. This analytical solution has been widely used to model solute or contaminant transport in fractured rocks at different scales, and employed to interpret laboratory experiments and field tracer tests.⁵ It was also widely adopted as the basic benchmark test tool for other specific mass transport and heat transfer problems in the fractured porous rocks.^{6–9}

In Ref. 2, the fracture was assumed to be formed by a pair of smooth parallel plates with a single-phase fluid flow of a constant velocity along the fracture, and the rock matrix was assumed to be a fully saturated porous medium of homogeneous porosity, with zero fluid velocity, in a 2D space. The transport processes in the fracture–matrix system were assumed to be governed by two coupled one-dimensional equations: one for the transport along the fracture and another for matrix diffusion in the direction perpendicular to the fracture length, by averaging the mass flux exchange at the fracture–matrix interface as a source term. In

order to derive the closed-form solutions of the equations, it was found that the transverse diffusion across the fracture fluid, longitudinal matrix diffusion in the direction along the fracture axis, and the difference of concentration gradient at the interface between fracture and matrix were ignored, by accepting three special assumptions, which are described in Section 3.2.

The impact of these special assumptions on modeling solute transport processes in rock fracture–matrix systems is an important issue, but has not previously been systematically evaluated. In practice, such impact may become important for modeling solute transport processes in fractured porous rock masses, for example, when using discrete fracture network models for problems of large spatial and long temporal scales. Therefore, a quantitative analysis for the impact of these special assumptions is needed. Roubinet et al.⁴ discussed the impact of transverse dispersion in fracture and longitudinal diffusion in matrix through semi-analytical solutions, and they found that the ratio of transverse dispersion in fracture and transverse diffusion in matrix are the key processes controlling the fracture–matrix exchange of solute masses. In addition, they found that the longitudinal diffusion in the matrix has impacts on the solute concentration in the fracture with low Péclet (Pe) numbers. The impact of these special assumptions, especially the assumption of constant concentration gradient at the interface between fracture and matrix, has not been checked against numerical modeling results. This issue motivated our research presented in this paper.

The aim of this study is to analyze and discuss the impacts of the special assumptions for deriving the analytical solution in Ref. 2 through numerical modeling, thus, to better understand and evaluate the uncertainties of modeling the solute transport

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processes in fractured rocks when analytical solutions are adopted as the basic mathematical tools.

2. Single fracture–matrix system

As presented in Ref. 2 we consider a conservative solute transport in a single fracture represented by a smooth parallel plate fracture model with a constant aperture $2b$, embedded in an semi-infinite and homogenously porous rock matrix, as shown in Fig. 1 as a conceptual model, where symbol C_m represents the solute concentration in the pore water of rock matrix, C_f represents solute concentration in fracture, u is the fluid velocity in the direction along the fracture and b is the half-aperture of the fracture, respectively.

Besides the simplified geometry of fracture–matrix system, the basic physical and mathematical assumptions, as adopted in Ref. 2 are: (1) the physical problem was defined in a 2D space; (2) the rock concerned is a homogenously porous rock with a small permeability, fully saturated but with zero fluid flow velocity; (3) the fluid flow in the fracture was assumed as laminar; (4) no mechanical and thermal processes were considered. For simplicity, only advection and dispersion in the fracture, and molecular diffusion in the matrix, were considered in this study, since our objectives are checking the impacts of the three special assumptions for deriving analytical solutions,² not a complete spectrum of the transport processes involved.

3. Governing equations and analytical solution

3.1. Solute transport equations

The solute transport processes in such a space of fracture–matrix system $\Omega = \{(x, z) : 0 \leq x < \infty, -\infty < z < \infty\}$, as shown in Fig. 1, can be expressed by a general transport equation without source terms, written as

$$\frac{\partial \theta C}{\partial t} + u \cdot \nabla C - \nabla \cdot \theta D (\nabla C) = 0 \tag{1}$$

where C (kg/m^3), t (s), u (m/s), D (m^2/s) and θ denote the volumetric solute concentration in fluid phase, the time, the fluid velocity, the dispersion coefficient and the rock matrix porosity, respectively.

For the fracture, the dispersion coefficient is given in Ref. 2 by

$$D = D_f = \alpha_L u + D^* \tag{2}$$

where α_L (m) is the longitudinal dispersivity along the fracture in the x -axis direction (Fig. 1), and D^* (m^2/s) is the molecular diffusion coefficient of solute in the fracture fluid (i.e. water). For the porous rock matrix, as $u=0$ was assumed, the dispersion coefficient is then equal to the effective diffusion coefficient D_m , and it was defined as

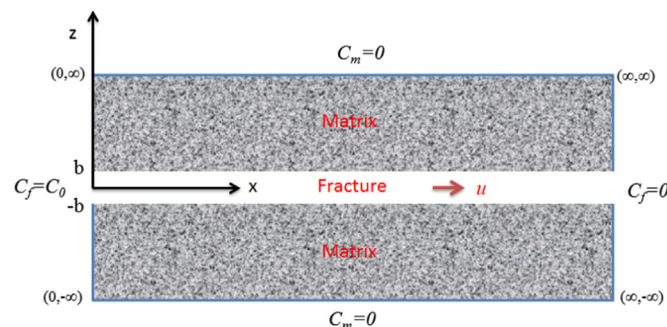


Fig. 1. Conceptual model of the fracture–matrix system geometry and boundary conditions.

related to the matrix tortuosity (τ), written as²

$$D = D_m = \tau D^* \tag{3}$$

Initially, no solute was assumed in the fracture–matrix system ($C = 0$ at $t = 0$). The boundary conditions are expressed as²

$$C(x=0, -b \leq z \leq b, t) = C_0, C(x=0, z < -b \text{ or } b < z, t) = 0,$$

$$C(x=\infty, z, t) = 0, C(x, z = \pm \infty, t) = 0 \tag{4}$$

3.2. Analytical solution by Tang et al.²

In order to analytically solve above transport equation in the fracture–matrix system, the general transport equation (Eq. 1) for the whole domain of the fracture–matrix system was often written as two separate transport equations: one for the fracture $\Omega_f = \{(x, z) : 0 \leq x < \infty, -b < z < b\}$ and another for the matrix $\Omega_m = \{(x, z) : 0 \leq x < \infty, b < z \text{ and } z < -b\}$. In Ref. 2, the two separate transport equations were simplified as two one-dimensional equations for solute transport in fracture and diffusion in matrix, respectively, by adopting the following special assumptions: (1) transverse diffusion and dispersion within the fracture assured full mixing across the fracture width (in the direction of the z -axis in Fig. 1) at all times; (2) the gradient of solute concentration at the interface in the direction of the z -axis ($\frac{\partial C_m(x)}{\partial z} |_{z=\pm b}$) was constant; (3) the matrix diffusion in the direction along the fracture length (in the direction of the x -axis in Fig. 1) was ignored. Note that the second assumption was implicitly required during the mathematical model setup process.

In order to demonstrate the mathematical model setup and requirements of these assumptions in Ref. 2, an illustration of mass conservation system in a differential control volume of the fracture is presented in Fig. 2. Only the first order of the solute fluxes was kept.

In Fig.2, $J_f(x)$ represents the solute flux in the the x -direction. It

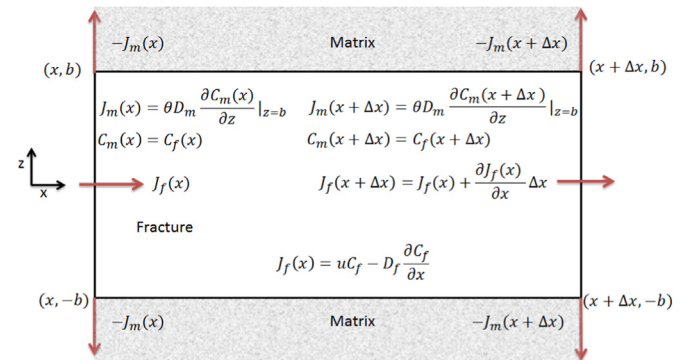


Fig. 2. Illustration of mass conservation in a differential control volume of fracture.

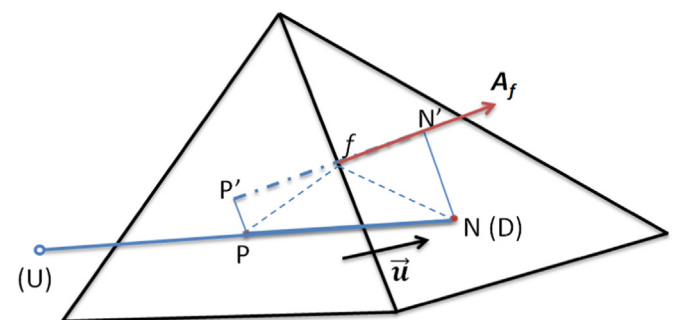


Fig. 3. Illustration of control volumes.

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