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Analytical solutions of solute transport in a fracture–matrix system with different reaction rates for fracture and matrix

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SUMMARY

This study deals with the problem of reactive solute transport in a fracture–matrix system using both analytical and numerical modeling methods. The groundwater flow velocity in the fracture is assumed to be high enough (no less than 0.1 m/day) to ensure the advection-dominant transport in the fracture. The problem includes advection along the fracture, transverse diffusion in the matrix, with linear sorption as well as first-order reactions operative in both the fracture and the matrix. A constant-concentration boundary condition and a decay source boundary condition in the fracture are considered. With a constant-concentration source, we obtain closed-form analytical solutions that account for the transport without reaction as well as steady-state solutions with different first-order reactions in the two media. With a decay source, a semi-analytical solution is obtained. The analytical and semi-analytical solutions are in excellent agreement with the numerical simulation results obtained using COMSOL Multiphysics. Sensitivity analysis is conducted to assess the relative importance of matrix diffusion coefficient, fracture aperture, and matrix porosity. We conclude that the first-order reaction as well as the matrix diffusion in the fractured rock would decrease the solute peak concentration and shorten the penetration distance into the fracture. The solutions can be applied to assess the spatial–temporal distribution of concentrations in the fracture and the matrix as well as to assess the contaminant mass stored in the rock matrix. All of these are useful for designing remediation plans for contaminated fractured rocks or for risk assessment of contaminated fracture–matrix systems.

1. Introduction

Studies on solute transport in fractured rocks are of great significance in many applications such as removing contaminants from fractured rocks and selecting repository sites for radioactive waste (Bodin et al., 2003; Lever and Bradbury, 1985; Neretnieks, 1980). In a fracture–matrix system, the permeability of the matrix may be several orders of magnitude less than that of the fracture and matrix advection is often neglected (Maloszewski and Zuber, 1993; Rasmuson and Neretnieks, 1981; Roubinet et al., 2012; Sudicky and Frind, 1982; Tang et al., 1981). In general, transport in fracture networks is conceptualized as advection through the fracture with diffusion into the surrounding rock matrix, with diffusion as the main transport mechanism in the matrix (Foster, 1975; Grisak and Pickens, 1980; Huyakorn et al., 1983; Park et al., 2001; Zhan et al., 2009). Some previous studies also found that matrix diffusion greatly affects the transport process and even could be a controlling factor in fracture transport when the matrix has a high value of porosity (Maloszewski and Zuber, 1985, 1990; Neretnieks, 1980; Sidle et al., 1998; Wendland and Himmelsbach, 2002).

Tang et al. (1981) first proposed a general analytical solution of contaminant transport through a water-saturated single fracture. Their controlling equations considered fracture dispersion and they compared the result to a solution which neglected fracture dispersion. As the comparison showed, the two solutions may differ in solute concentration profile with a lower groundwater velocity (0.01 m/d). However, the difference would not be significant when the velocity was relatively high (0.1 m/d) (Tang et al., 1981; Sudicky and Frind, 1982). In fact, groundwater velocity is higher than the value of 0.1 m/d in some actual situations (Ge, 1998; Novakowski et al., 2006). Similarly, Roubinet et al. (2012) concluded that longitudinal and transverse dispersion in the fracture would insignificantly affect the transport in a fractured rock system when the fracture flow velocity is high (the value consid-

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ered in their study was 0.86 m/d). Roubinet et al. (2012) further studied the effects on transport by transverse dispersion in the fracture and longitudinal diffusion in the matrix. They found that fracture transverse dispersion had little impact on the transport processes in a classical fracture–matrix system (in which the fracture transverse dispersion coefficient is larger than the matrix transverse diffusion coefficient) and longitudinal diffusion in the matrix obviously impacts the transport only when the Peclet number was low (no more than 10^{-2}). Sudicky and Frind (1982) extended the previous work (Tang et al., 1981) by developing an exact analytical solution of a set of identical parallel fractures. Cook and Robinson (2002) modified the solution of Sudicky and Frind (1982) using a specified flux upper boundary condition. Both studies used no-flux boundary conditions midway between the fractures. This is inappropriate in applying to the real conditions where the fractures have different boundary conditions, apertures and other hydraulic properties.

First-order reaction refers to the reaction whose rate is proportional to the concentration of reactant. It may include some natural decays of radioactive or biological species, degradations and biodegradations. Tang et al.'s (1981) work considered the natural decay term and used identical decay constants in the fracture and the matrix. Nevertheless, it is likely to have different reaction rate constants in the two media. For example, biodegradation reaction would be influenced by water temperature, type and content of organic compound, oxygen concentration and many other factors (Brakstad and Bonaunet, 2006; Davis et al., 2013; Johnson and Furrer, 2002; Kim et al., 2013). Some of those factors may be different in the fracture and the matrix. Therefore, it is necessary to take into account different first-order reaction rates in a fracture–matrix system.

In this study, we use an analytical model to describe transport in a fracture–matrix system with relatively high groundwater flow velocity in the fracture, neglecting fracture longitudinal dispersion and rock matrix advection. This work differs from previous studies by considering different first-order reaction rates in the fracture and matrix. Other new features of this study are as follows. A finite-element numerical simulation is presented using COMSOL Multiphysics for the sake of comparison with the developed analytical and semi-analytical solutions. Sensitivity analysis is conducted to identify the primary factors controlling the transport process. With the obtained solutions, one could compute the total solute mass as well as final plume size, which will be helpful for designing remediation plan for cleaning up contaminated fracture–matrix systems or for risk assessment of such systems in terms of long time environmental impact.

2. Conceptual and mathematical models

2.1. Conceptual model

The transport process investigated here takes place in a single fracture, adjacent with a rock matrix which has much smaller permeability as compared to the fracture (Fig. 1). The rock matrix is assumed to be thick enough so that its other boundary will not affect the solute transport. In addition, the fracture (or the matrix) is assumed to have homogeneous transport properties with a constant flow velocity. The fracture aperture is assumed to be uniform over the domain of investigation. Advective transport occurs in the fracture and transverse diffusion occurs in the matrix. Solute diffusion occurs at the interface of the two media. We also assume that the flow is driven by a simple uniform pressure gradient aligned with the fracture axis so that the velocity in the fracture has a constant value. The origin of coordinate system is at the left boundary in the middle of the fracture. The x axis is along the groundwater flow direction in the fracture (horizontal) and the z axis is upward (vertical).

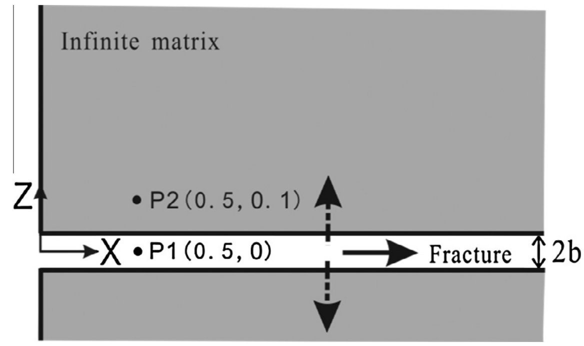

Fig. 1. Schematic diagram of the fracture–matrix system.

We will consider two kinds of boundary conditions for the source at $x = 0$. The first is a constant-concentration source, which is commonly used in solute transport studies (Batu, 1996; Roubinet et al., 2012; Tang et al., 1981). The other boundary condition is a decay source, which is relevant to radioactive waste transport (Moreno et al., 2006; Park et al., 2001; Shahkarami et al., 2015). In accordance with above constrains, a mathematical model is established as follows.

2.2. Mathematical model and solutions

2.2.1. Non-reaction case with a constant-concentration source

First we will develop a transport model without reactions and with a constant-concentration source. The governing equations and the initial and boundary conditions can be described as follows. For the fracture,

$$\frac{\partial C_f}{\partial t} = -V\frac{\partial C_f}{\partial x} - \frac{q}{b}, \tag{1}$$

$$q = -n_m D_d \frac{\partial C_m}{\partial z}\bigg|_{z=b}, \tag{2}$$

$$C_f(x=0,t) = C_0, \tag{3}$$

$$C_f(x,t=0) = 0. \tag{4}$$

And for the matrix,

$$\frac{\partial C_m}{\partial t} = D_d \frac{\partial^2 C_m}{\partial z^2}, \tag{5}$$

$$C_m(x,z=b,t) = C_f(x,t), \tag{6}$$

$$C_m(x,z=\infty,t) = 0, \tag{7}$$

$$C_m(x,z,t=0) = 0, \tag{8}$$

where C_f represents solute concentration in the fracture and C_m represents solution concentration in the matrix; C_0 is the source concentration (constant); V is the groundwater flow velocity in the fracture (constant); x and z are the horizontal and vertical coordinates, respectively; t is time since the release of the contaminant; q is the diffusive mass flux in the upper or lower rock matrix adjacent to the fracture; n_m is the porosity; D_d is the effective diffusion coefficient, which equals to τD_0; τ and D_0 are the matrix tortuosity (between 0 and 1) and the molecular diffusion coefficient in free solution, respectively; b is the fracture half aperture or $2b$ is the fracture aperture (constant). First we apply Laplace transform to the governing equations and boundary conditions and obtain solu-